

Interacting bosons in an optical lattice

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Several models of a strongly interacting Bose gas in an optical lattice are studied within the functional-integral approach. The one-dimensional Bose gas is briefly discussed. Then the Bose-Einstein condensate and the Mott insulator of a three-dimensional Bose gas are described in mean-field approximation, and the corresponding phase diagrams are evaluated. Other characteristic quantities, like the spectrum of quasiparticle excitations and the static structure factor, are obtained from Gaussian fluctuations around the mean-field solutions. We discuss the role of quantum and thermal fluctuations, and determine the behavior of physical quantities in terms of density and temperature of the Bose gas. In particular, we study the dilute limit, where the mean-field equation becomes the Gross-Pitaevskii equation. This allows us to extend the Gross-Pitaevskii equation to the dense regime by introducing renormalized parameters in the latter.

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1 Introduction

The quantum statistics of non-interacting particles was established by S. N. Bose in 1924 [1]. Bose was able to deduce Planck's radiation law on the assumption that each quantum state can be occupied by an arbitrary number of indistinguishable photons. By applying this idea to the quantum statistics of an ideal gas of N_{tot} atoms enclosed in a volume V , A. Einstein predicted the occurrence of a phase transition [2]: Below a critical temperature T_c , a certain fraction of atoms would "condense" in the ground state of the system. This phenomenon is called Bose-Einstein condensation (BEC).

In a homogeneous ideal Bose-gas (i.e., in the absence of an external potential), the critical temperature of the ideal Bose gas is given as [3, 4, 5, 6, 7]

$$k_B T_c = \frac{2\pi\hbar^2}{m} \left(\frac{n_{\text{tot}}}{\zeta\left(\frac{3}{2}\right)} \right)^{\frac{2}{3}}, \quad (1)$$

where k_B is Boltzmann's constant, \hbar is the reduced Planck's constant, $n_{\text{tot}} = N/V$ is the particle density, m is the mass of the particles, and $\zeta(x)$ is Riemann's Zeta-Function. The condensate fraction is given as

$$\frac{n_0}{n_{\text{tot}}} = \begin{cases} 0 & \text{if } T > T_c \\ 1 - \left(\frac{T}{T_c}\right)^{\frac{3}{2}} & \text{if } T < T_c \end{cases}, \quad (2)$$

where n_0 is the condensate density.

Historically, the first candidate for a possible realization of Bose-Einstein condensation was superfluid ^4He , discovered by P. L. Kapitza in 1934 below $T_c = 2.2\text{K}$. Although superfluid Helium is far away from the ideal Bose gas considered by Einstein because of strong interactions between the Helium atoms, the phenomena of superfluidity and BEC are related. Superfluidity was first explained by L. D. Landau in 1941 by an argument which is based on the idea that the viscosity of a fluid depends on the existence of quasiparticle excitations. Those excitations are created by friction between the fluid and a wall of the container. When the fluid has a velocity \mathbf{v} relative to the wall, these excitations are relevant only if their creation at momentum \mathbf{k} is energetically profitable, i. e. if the excitation energy is negative [4]:

$$E_{\mathbf{k}} + \hbar\mathbf{k} \cdot \mathbf{v} < 0.$$

Here $E_{\mathbf{k}}$ is the quasiparticle spectrum. In other words, the superfluid is destroyed by excitations if the velocity $|\mathbf{v}|$ exceeds a critical value v_c with

$$v_c = \min_{\mathbf{k}} \frac{E_{\mathbf{k}}}{\hbar k},$$

where the minimum is calculated over all the values of \mathbf{k} . If the spectrum is linear for small momenta, a non-zero value of v_c is found. It is important to notice that superfluidity and BEC are not identical. For instance, an ideal Bose gas can condense, but it is not superfluid due to Landau's principle, because the excitation spectrum is quadratic in k and therefore v_c is zero. On the other hand, a weakly-interacting two-dimensional Bose gas satisfies Landau's criterion for superfluidity, but long-range order cannot appear due to the Mermin-Wagner theorem [8, 9, 10], therefore there is no BEC.

In an interacting Bose gas of uncharged atoms, the main contribution to the interparticle interaction comes from s -wave scattering between two particles. The characteristic length scale here is the scattering length a_s . We assume a_s to be positive, although it can also be negative in trapped Bose gases (without trapping potential a Bose gas with negative a_s is unstable [4]). For theoretical description, usually two-body interaction is assumed. Approximately, the two-body interaction potential can be written in the form of a δ -potential:

$$V_{\text{int}}(\mathbf{r} - \mathbf{r}') \approx g \delta(\mathbf{r} - \mathbf{r}'). \quad (3)$$

Here, g is the strength of the repulsive interaction between two bosons. It is connected to the s -wave scattering length by the relation [4]

$$g = \frac{4\pi a_s \hbar^2}{m} . \quad (4)$$

This approximation is justified if the a_s is small compared to the thermal de Broglie wavelength, the inter-particle spacing, and the characteristic length scale of the trapping potential [5]. It is possible to tune the scattering length over a large range of values (positive as well as negative) to reach the strongly interacting regime, where Bogoliubov theory is not applicable anymore [4, 11, 12]. These magnetic Feshbach resonances became possible after the development of optical trapping as an alternative to magnetic trapping.

After the introduction of an external potential V_{ext} , the full Hamiltonian of the Bose system in terms of bosonic field operators is

$$\hat{H} = \int d^3r \left[\hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right) \hat{\psi}(\mathbf{r}) + \frac{g}{2} \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right] . \quad (5)$$

The ground state of this interacting many-body system is not known, therefore the condensate density cannot be defined by the population density of the ground state like in the ideal Bose gas. An appropriate definition for a homogeneous system is the concept of “off-diagonal long-range order” which was developed in the 1950’s [4, 5, 13]. The condensate density is given by the long-range behavior of the one-particle correlation function

$$n_0 := \lim_{\mathbf{r} \rightarrow \mathbf{r}'} \langle \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') \rangle . \quad (6)$$

If the one-particle correlation function decays exponentially or algebraically, the condensate density is zero. An algebraic decay is found in a two-dimensional Bose gas at low temperature and in a one-dimensional Bose gas at zero temperature [14].

1.1 Dilute Bose gas

When the mean distance between atoms is large compared to their scattering length, which is the case when $n_{\text{tot}} a_s^3 \ll 1$, the system is said to be in the dilute regime. In this case, the effect of interaction is small. A consistent mean-field theory of a dilute Bose gas which is valid for low temperatures $T \ll T_c$ was given by N. N. Bogoliubov in 1947 [3, 4]. The condensed phase is described by replacing the bosonic field-operators by the sum of a complex condensate order parameter Φ_0 and fluctuations out of the condensate as

$$\hat{\psi}(\mathbf{r}, t) = \Phi_0(\mathbf{r}, t) + \tilde{\psi}(\mathbf{r}, t) , \quad (7)$$

where the field operators $\tilde{\psi}$ of the fluctuations fulfill bosonic commutation relations. This theory gives elementary excitations out of the condensate which have the energy spectrum

$$E_{\mathbf{k}} = \sqrt{\frac{\hbar^2 k^2}{2m} \left(2gn_0 + \frac{\hbar^2 k^2}{2m} \right)} \quad (8)$$

where \mathbf{k} is the wave vector. It is linear for small momenta (“phonon spectrum”) and therefore satisfies Landau’s criterion for superfluidity, in contrast to Einstein’s non-interacting Bose gas with a quadratic energy spectrum. An important feature of an interacting Bose gases is the ground state depletion, which means that even at $T = 0$ the condensate fraction is smaller than 1. This is also found in Bogoliubov theory. In a dilute Bose gas, the condensate depletion is small.

The condensate order parameter Φ_0 is connected to the breaking of the global $U(1)$ symmetry, which reflects the fact that the replacement

$$\Phi_0(\mathbf{r}, t) \rightarrow e^{i\alpha} \Phi_0(\mathbf{r}, t) , \quad (9)$$

where α is a global phase, does not change the physics of the system. The phase α can be chosen arbitrarily, but once it has been chosen, the symmetry is broken. This is the case in the BEC phase. This phase α is responsible for the fact that the quasiparticle spectrum in Eq. (8) vanishes for $\mathbf{k} = 0$: The Goldstone-theorem states that the existence of a broken $U(1)$ phase symmetry leads to a gapless excitation spectrum [15].

The order parameter is interpreted as a macroscopic wave function and can be split into its modulus and phase:

$$\Phi_0(\mathbf{r}, t) = |\Phi_0(\mathbf{r}, t)| e^{i\theta(\mathbf{r}, t)}. \quad (10)$$

The local condensate density is related to the modulus squared of the order parameter

$$n_0(\mathbf{r}, t) = |\Phi_0(\mathbf{r}, t)|^2, \quad (11)$$

and the gradient of its phase, $\nabla\theta(\mathbf{r}, t)$, is associated with the velocity field of the condensed atoms. Gross and Pitaevskii have independently derived an equation to describe the dynamics of the order parameter, which is known as the Gross-Pitaevskii (GP) equation [4, 6, 5]:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Phi_0(\mathbf{r}, t)|^2 \right) \Phi_0(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \Phi_0(\mathbf{r}, t). \quad (12)$$

The third order term in Φ_0 , which is proportional to the interaction constant g , can be interpreted as the coupling of the order parameter to the local particle density as given in Eq. (11). For stationary solutions of the GP equation we use the ansatz $\Phi_0(\mathbf{r}, t) = \Phi_0(\mathbf{r}) \exp(-i\mu t/\hbar)$, where μ is the chemical potential. The GP equation then reduces to the stationary form

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) - \mu + g|\Phi_0(\mathbf{r})|^2 \right) \Phi_0(\mathbf{r}) = 0. \quad (13)$$

1.2 Trapped Bose gas

The experimental realisation of a weakly interacting BEC in a magnetic trap achieved in 1995 by E. Cornell and C. Wiemann at Boulder and W. Ketterle at MIT in vapors of ^{87}Rb ($a_s = 5.77\text{nm}$) and ^{23}Na ($a_s = 2.75\text{nm}$). This became possible by a combination of evaporative cooling and laser cooling. These systems are well described by Bogoliubov theory and the GP equation.

For models of the trapped condensates as those realized in experiments, usually a harmonic trap potential of the general form

$$V_{\text{ext}}(\mathbf{r}) = V_{\text{tr}}(\mathbf{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (14)$$

is assumed. For an ideal Bose gas, the critical temperature is given as [4]

$$k_B T = \hbar \omega_{\text{ho}} \left(\frac{N_{\text{tot}}}{\zeta(3)} \right)^{\frac{1}{3}}, \quad \omega_{\text{ho}} = (\omega_x \omega_y \omega_z)^{\frac{1}{3}}, \quad (15)$$

in contrast to the critical temperature of a homogeneous BEC in Eq. (1). Instead of Eq. (2), the condensate fraction in a trapped condensate is

$$\frac{n_0}{n_{\text{tot}}} = \begin{cases} 0 & \text{if } T > T_c \\ 1 - \left(\frac{T}{T_c} \right)^3 & \text{if } T < T_c \end{cases}. \quad (16)$$

In rotating BECs, quantized vortices and vortex lattices have been observed, a phenomenon which is also known in type-II superconductors and superfluid ^4He [16, 17]. Vortices are observed by absorption imaging [18].

If the condensate is in rotational equilibrium at angular velocity Ω around the z -axis, the critical angular velocity Ω_c , at which the creation of a vortex occurs, as well as the stability and dynamics of vortex cores and vortex lattices have, can be calculated by minimizing the free energy within the GP approach [19, 20, 21, 22, 23].

1.3 Light scattering and structure factor

Light scattering experiments on BECs allow the study of density fluctuations. In so-called Bragg scattering experiments, light scattering is studied as a stimulated process, induced by two laser beams which illuminate the atomic sample [24]. In scattering events elementary excitations are created, and the momentum and energy transfer is pre-determined by the angle and frequency difference between the incident beams.

The most important quantity here is the dynamic structure factor $S(\mathbf{q}, \omega)$, which is proportional to the excitation rate per particle. Here, $\mathbf{q} = \mathbf{q}_f - \mathbf{q}_i$, and \mathbf{q}_i is the wave vector of the incoming, \mathbf{q}_f is the wave vector of the reflected light beam, and ω is the frequency difference between the two laser beams.

The dynamic structure factor describes a correlation between a density fluctuation at time $t_0 = 0$ and at time $t_1 = t$ and is defined as the expectation value [25]

$$S(\mathbf{q}, \omega) = \frac{1}{N_{\text{tot}}} \int \langle \hat{\rho}_{\mathbf{q}}(t) \hat{\rho}_{\mathbf{q}}^+(0) \rangle e^{i\omega t} dt, \quad (17)$$

with the density operator in momentum space, which is given as

$$\hat{\rho}_{\mathbf{q}}^+ = \int \hat{n}_{\mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{r}} d^d r = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}+\mathbf{q}}^+ \hat{a}_{\mathbf{k}}, \quad (18)$$

in Schrödinger representation and

$$\hat{\rho}_{\mathbf{q}}(t) = e^{-i(\hat{H} - \mu \hat{N})t/\hbar} \hat{\rho}_{\mathbf{q}} e^{i(\hat{H} - \mu \hat{N})t/\hbar}. \quad (19)$$

in Heisenberg representation, where $\hat{a}_{\mathbf{k}}$, $\hat{a}_{\mathbf{k}}^+$ fulfil bosonic commutation relations. Integrating over all frequencies ω one obtains the static structure factor

$$S(\mathbf{q}) = \int S(\mathbf{q}, \omega) d\omega, \quad (20)$$

which is equivalent to the line strength of the Bragg resonance. The static structure factor is then given by Eq. (20) as

$$S(\mathbf{q}) = \frac{1}{N_{\text{tot}}} \langle \hat{\rho}_{\mathbf{q}}(0) \hat{\rho}_{\mathbf{q}}^+(0) \rangle. \quad (21)$$

In the ground state of a non-interacting condensate, the static structure factor is unity, and in the Bogoliubov ground state, it is given as

$$S(\mathbf{q}) = \frac{\hbar^2 \mathbf{q}^2}{2m E_{\mathbf{q}}}, \quad (22)$$

where $E_{\mathbf{q}}$ is the quasiparticle spectrum given in (8). This result has been originally derived by R. Feynman for the static structure factor of superfluid ⁴He [26], and will be reproduced in chapter 4. In the regime of long wave lengths this becomes

$$S(\mathbf{q}) = \frac{\hbar |\mathbf{q}|}{2mc} + \mathcal{O}(q^2), \quad (23)$$

where c is the sound velocity.

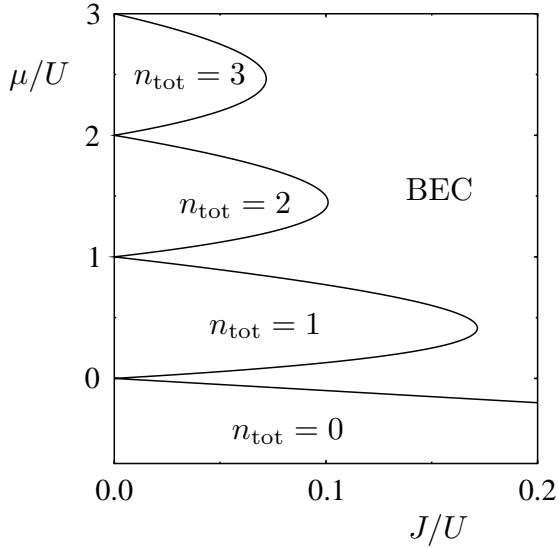


Fig. 1 Zero temperature phase diagram of the Bose-Hubbard model calculated in mean-field theory.

1.4 Optical lattices

Recently, ultracold gases were superimposed by optical lattices, which are created by standing waves of laser fields [27]. There are one-, two- and three-dimensional optical lattices. The lattice potential of a three-dimensional cubic optical lattice created of three perpendicular laser beams parallel to the coordinate axes, is of the general form

$$V_{\text{latt}}(\mathbf{r}) = V_x \sin^2(q_0 x) + V_y \sin^2(q_0 y) + V_z \sin^2(q_0 z), \quad (24)$$

where the amplitudes V_x , V_y , V_z are proportional to the intensity of the laser field. Together with the harmonic trap potential given in Eq. (14) the external potential of the atoms is $V_{\text{ext}}(\mathbf{r}) = V_{\text{tr}}(\mathbf{r}) + V_{\text{latt}}(\mathbf{r})$.

A one-dimensional Bose gas, where the movement of atoms is only possible in one direction (e.g. the z -direction), can be created by tightly confining the particle motion in two directions (the x - and y -direction) to zero point oscillations. This can be done by increasing the amplitude V_x and V_y until tunneling of atoms through the lattice wells is prohibited. If $V_z = 0$, the Bose gas is trapped in one-dimensional tubes, and if $V_z \neq 0$ but small compared to V_x and V_y , a one-dimensional lattice is created where atoms can only tunnel between neighboring lattice-sites in the z -direction [28].

The conventional model for a single-component system of bosons in an optical lattice is the Bose-Hubbard model. Assuming a d -dimensional simple-cubic lattice potential with $q_x = q_y = q_z \equiv q$ and $V_x = V_y = V_z \equiv V_0/3$, it has the form [29, 30, 31]

$$\hat{H}_{\text{BH}} = -\frac{J}{2d} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{a}_{\mathbf{r}}^{\dagger} \hat{a}_{\mathbf{r}'} + \sum_{\mathbf{r}} V_{\mathbf{r}} \hat{a}_{\mathbf{r}}^{\dagger} \hat{a}_{\mathbf{r}} + \frac{U}{2} \sum_{\mathbf{r}} \hat{a}_{\mathbf{r}}^{\dagger} \hat{a}_{\mathbf{r}}^{\dagger} \hat{a}_{\mathbf{r}} \hat{a}_{\mathbf{r}}, \quad (25)$$

where \mathbf{r}, \mathbf{r}' denote the discrete positions of the lattice sites, \hat{a} and \hat{a}^{\dagger} are bosonic annihilation and creation operators and the sum of the kinetic term runs over nearest neighbor sites only. The position \mathbf{r}_i of site i is at a minimum of the lattice potential, i.e. $V_{\text{latt}}(\mathbf{r}_i) = 0$.

The Bose-Hubbard model can describe a new phase, the Mott-insulator (MI). It is characterized by a complete loss of phase coherence between different lattice sites and an integer number of bosons at each

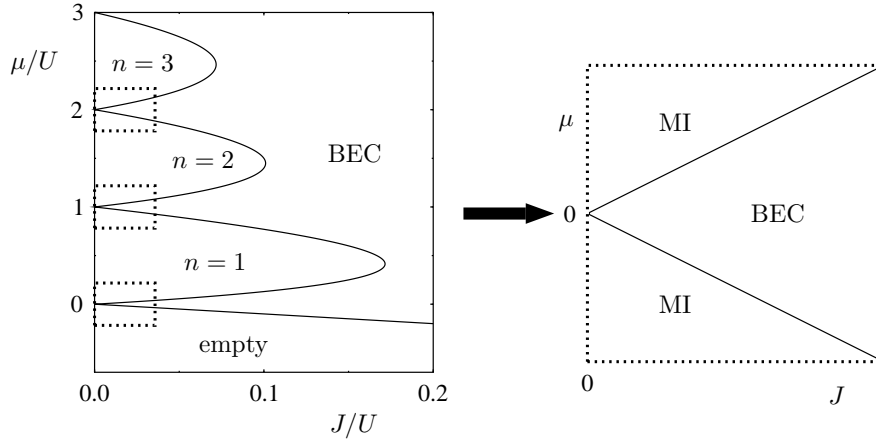


Fig. 2 A projection of the phase diagram of the Bose-Hubbard model in the vicinity of the point, where the two Mott lobes meet. μ and J are in arbitrary energy units after the projection.

lattice site (“lobes” in the phase diagram in Fig. 1). The loss of phase coherence has been shown in experiments [27]. The MI is favored if the on-site interaction U dominates the hopping J .

In the hard-core boson model, which will be discussed in the following sections, each lattice site cannot be occupied by more than one boson. Contrary, the Bose-Hubbard model which allows multiple occupation to the price of the interaction energy U . The existence of BEC phase in the three-dimensional hard-core boson model has been proven rigorously [32].

The Hamiltonian of the hard-core boson model can be written in terms of creation and annihilation operators $\hat{a}_{\mathbf{r}}^+$ and $\hat{a}_{\mathbf{r}}$ with the usual bosonic commutation relations $[\hat{a}_{\mathbf{r}}, \hat{a}_{\mathbf{r}'}^+] = 0$ for different sites $\mathbf{r} \neq \mathbf{r}'$. They have the additional hard-core property

$$\hat{a}_{\mathbf{r}}^2 = (\hat{a}_{\mathbf{r}}^+)^2 = 0, \quad (26)$$

which limits the occupation number at lattice site \mathbf{r} to 0 and 1. With those operators, the Hamiltonian is [33, 34]

$$\hat{H}_{\text{hc}} = -\frac{J}{2d} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{a}_{\mathbf{r}}^+ \hat{a}_{\mathbf{r}'} + \sum_{\mathbf{r}} V_{\mathbf{r}} \hat{a}_{\mathbf{r}}^+ \hat{a}_{\mathbf{r}}. \quad (27)$$

The hard-core boson model can be understood as a projection of the more general Bose-Hubbard model in the vicinity of those points of the phase diagram, where two adjacent Mott lobes meet (Fig. 2). This is similar to the picture which was applied to the tips of the Mott lobes in a recent paper by Huber et al. [35]. It is based on the following idea. The number of bosons per site is fixed in the Mott state. For adjacent Mott lobes this means that the corresponding Mott states differ exactly by one boson per site. Now we consider two adjacent lobes with n and $n+1$ ($n \geq 0$ bosons per site), respectively and assume that the chemical potential is fixed such that the ground state is the Mott state with n particles per site. Low-energy excitations of this state for a grand-canonical system are states, where one or a few sites (e.g. $k \geq 1$ sites) have $n+1$ bosons, all other sites have n bosons. The k excessive bosons are relatively free to move from site to site on top of the n Mott state. Therefore, the physics of these excitations can be described approximately by the tunneling of the k excessive bosons alone. Due to the repulsion of order U , assumed to be not too small, it is unlikely that a site with $n+2$ bosons is created. Consequently, these excessive bosons form a hard-core Bose gas.

1.5 Outline of the following sections

In section 2 the functional integral representation is introduced in the form as it is applied to the models which are reviewed. It is shown that all physical quantities can be derived from the functional integral representation of the grand canonical partition function.

In section 3, exactly solvable models are presented, namely the ideal Bose gas and a one dimensional hard-core Bose gas on an optical lattice. Section 4 presents a summary of the results of the weakly interacting Bose gas on the level of Gaussian fluctuations around the mean-field solutions. It leads to the well-known results of Bogoliubov theory. Two approaches to the dense regime of strongly interacting bosons are provided in section 5. The first one will be called the paired-fermion model, and the second is based on the slave-boson approach.

2 Functional integral method

2.1 Grand canonical partition function as functional integral

The grand canonical partition function Z of a many-body system contains all information about the thermodynamic equilibrium properties of that system [3]. For given Hamiltonian \hat{H} it is given as the trace of the density operator ρ :

$$\hat{\rho} = e^{-\beta(\hat{H} - \mu\hat{N}_{\text{tot}})}, \quad Z = \text{Tr}(\hat{\rho}) \quad (28)$$

Here, $\beta = 1/(k_B T)$ is the inverse temperature, μ is the chemical potential and the particle number operator is $\hat{N}_{\text{tot}} = \sum_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}$. It is possible to write a grand canonical partition function in terms of a functional integral [36, 14].

2.1.1 Bosonic functional integral

Consider a bosonic many-body system given by the Hamiltonian $\hat{H}(\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha})$, where the creation and annihilation operators $\hat{a}_{\alpha}^{\dagger}$ and \hat{a}_{α} fulfil bosonic commutation relations:

$$[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}]_{-} = \delta_{\alpha\beta}; \quad [\hat{a}_{\alpha}, \hat{a}_{\beta}]_{-} = [\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\beta}^{\dagger}]_{-} = 0. \quad (29)$$

The index α denotes the states $|\alpha\rangle$ of an arbitrary single-particle basis, e.g. α can denote a lattice site or a wave vector. The grand canonical partition function is given as a functional integral over the complex field ϕ :

$$Z = \lim_{M \rightarrow \infty} \int e^{-A(\phi^*, \phi)} \prod_{n=1}^M \prod_{\alpha} \frac{d\phi_{\alpha,n}^* d\phi_{\alpha,n}}{2\pi i} \quad (30)$$

with the action

$$A(\phi^*, \phi) = \frac{\beta}{M} \sum_{n=1}^M \left\{ \sum_{\alpha} \phi_{\alpha,n+1}^* \left[\frac{M}{\beta} (\phi_{\alpha,n+1} - \phi_{\alpha,n}) - \mu \phi_{\alpha,n} \right] + H(\phi_{\alpha,n+1}^*, \phi_{\alpha,n}) \right\}. \quad (31)$$

We require for bosons the periodic boundary conditions $\phi_{\alpha,1} = \phi_{\alpha,M+1}$ and $\phi_{\alpha,1}^* = \phi_{\alpha,M+1}^*$. The function $H(\phi_{\alpha,n+1}^*, \phi_{\alpha,n})$ is obtained from the Hamiltonian $\hat{H}(\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\alpha})$ by making the replacements $\hat{a}_{\alpha}^{\dagger} \rightarrow \phi_{\alpha,n+1}^*$ and $\hat{a}_{\alpha} \rightarrow \phi_{\alpha,n}$. After performing the limit $M \rightarrow \infty$, n plays the role of a continuous imaginary time variable. Using $\tau := n\hbar\beta/M$ we can write

$$Z = \int e^{-A(\phi^*, \phi)} \mathcal{D}(\phi^*(\tau)\phi(\tau)), \quad \mathcal{D}(\phi^*(\tau)\phi(\tau)) := \lim_{M \rightarrow \infty} \prod_{n=1}^M \prod_{\alpha} \frac{d\phi_{\alpha,n}^* d\phi_{\alpha,n}}{2\pi i} \quad (32)$$

and

$$A(\phi^*, \phi) = \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left\{ \sum_{\alpha} \phi_{\alpha}^*(\tau) \left(\hbar \frac{\partial}{\partial \tau} - \mu \right) \phi_{\alpha}(\tau) + H(\phi_{\alpha}^*(\tau), \phi_{\alpha}^*(\tau)) \right\}. \quad (33)$$

In the following we keep M finite during the calculations and the limit $M \rightarrow \infty$ is performed in the end.

2.1.2 Fermionic functional integral

In the case of a fermionic many-body Hamiltonian $\hat{H}(\hat{c}_{\alpha}^{\dagger}, \hat{c}_{\alpha})$, the creation and annihilation operators fulfil the anti-commutation relations

$$[\hat{c}_{\alpha}, \hat{c}_{\beta}^{\dagger}]_{+} = \delta_{\alpha\beta}; \quad [\hat{c}_{\alpha}, \hat{c}_{\beta}]_{+} = [\hat{c}_{\alpha}^{\dagger}, \hat{c}_{\beta}^{\dagger}]_{+} = 0. \quad (34)$$

A functional integral of a fermionic system is given as an integral of conjugate Grassmann variables. The definition of a Grassmann algebra can be found in refs. [36, 14, 37]. Here it shall only be mentioned that the variables of conjugate Grassmann fields $\bar{\psi}, \psi$ are anti-commuting, i. e.

$$\psi_{\alpha,n} \psi_{\beta,m} = -\psi_{\beta,m} \psi_{\alpha,n}, \quad \bar{\psi}_{\alpha,n} \bar{\psi}_{\beta,m} = -\bar{\psi}_{\beta,m} \bar{\psi}_{\alpha,n}, \quad \bar{\psi}_{\alpha,n} \psi_{\beta,m} = -\psi_{\beta,m} \bar{\psi}_{\alpha,n},$$

and a Grassmann integral gives unity only if it is performed over a full product of all variables, and zero otherwise:

$$\int \bar{\psi}_{\alpha,n} \psi_{\alpha,n} d\psi_{\alpha,n} d\bar{\psi}_{\alpha,n} = 1, \quad (35)$$

$$\int d\psi_{\alpha,n} d\bar{\psi}_{\alpha,n} = \int \bar{\psi}_{\alpha,n} d\psi_{\alpha,n} d\bar{\psi}_{\alpha,n} = \int \psi_{\alpha,n} d\psi_{\alpha,n} d\bar{\psi}_{\alpha,n} = 0. \quad (36)$$

Using these rules, the functional integral of the fermionic grand canonical partition function can be constructed by analogy with Eq. (30) as

$$Z = \lim_{M \rightarrow \infty} \int e^{-A(\bar{\psi}, \psi)} \prod_{n=1}^M \prod_{\alpha} d\bar{\psi}_{\alpha,n} d\psi_{\alpha,n}. \quad (37)$$

In the action (31), the complex variables $\phi_{\alpha,n}^*, \phi_{\alpha,n}$ have to be replaced by the Grassmann variables $\bar{\psi}_{\alpha,n}, \psi_{\alpha,n}$, and the periodic boundary conditions have to be replaced by anti-periodic boundary conditions $\psi_{\alpha,1} = -\psi_{\alpha,M+1}$ and $\bar{\psi}_{\alpha,1} = -\bar{\psi}_{\alpha,M+1}$. The same replacements can be done in the imaginary time functional integral defined by Eqs. (32) and (33), then the integration measure in (32) is replaced by

$$\mathcal{D}(\bar{\psi}(\tau) \psi(\tau)) := \lim_{M \rightarrow \infty} \prod_{n=1}^M \prod_{\alpha} d\bar{\psi}_{\alpha,n} d\psi_{\alpha,n} \quad (38)$$

for the Grassmann fields. (For the construction of the functional integral for bosons and fermions with coherent states see Appendix B)

2.2 Correlation functions

Physical quantities can be written in terms of expectation values. The expectation value of an arbitrary operator \hat{X} is given by the relation

$$\langle \hat{X} \rangle = \frac{1}{Z} \text{Tr} \left(\hat{X} \hat{\rho} \right) \quad (39)$$

with the density operator (28). The general static n -particle correlation function (CF) is defined as a product of n creation and n annihilation operators:

$$C_n(\alpha_1, \dots, \alpha_n; \beta_n, \dots, \beta_1) := \langle \hat{a}_{\alpha_1}^+ \cdots \hat{a}_{\alpha_n}^+ \hat{a}_{\beta_n} \cdots \hat{a}_{\beta_1} \rangle. \quad (40)$$

In the functional integral representation of a bosonic system, an expectation value of some function $f(\phi^*, \phi)$, which depends on the complex field variables, is defined as

$$\langle f(\phi^*, \phi) \rangle = \frac{1}{Z} \int f(\phi^*, \phi) e^{-A(\phi^*, \phi)} \mathcal{D}(\phi^*(\tau) \phi(\tau)). \quad (41)$$

Note that in a fermionic system, the complex fields have to be replaced by Grassmann fields, otherwise there is no difference in the formalism. To translate the static CF (40) to an expectation value in terms of a functional integral, it is necessary to introduce a dynamic n -particle CF, which depends on the imaginary time variable τ . Therefore we introduce the imaginary time Heisenberg representation of the bosonic creation and annihilation operators \hat{a}_α^+ and \hat{a}_α :

$$\hat{a}_\alpha^+(\tau) = e^{\tau(\hat{H} - \mu \hat{N}_{\text{tot}})/\hbar} \hat{a}_\alpha^+ e^{-\tau(\hat{H} - \mu \hat{N}_{\text{tot}})/\hbar} \quad (42)$$

$$\hat{a}_\alpha(\tau) = e^{\tau(\hat{H} - \mu \hat{N}_{\text{tot}})/\hbar} \hat{a}_\alpha e^{-\tau(\hat{H} - \mu \hat{N}_{\text{tot}})/\hbar}. \quad (43)$$

The dynamic n -particle CF can now be defined as

$$C_n(\alpha_1 \tau_1, \dots, \alpha_n \tau_n; \beta_n \tau_{n+1}, \dots, \beta_1 \tau_{2n}) := \langle \hat{a}_{\alpha_1}^+(\tau_1) \cdots \hat{a}_{\alpha_n}^+(\tau_n) \hat{a}_{\beta_n}(\tau_{n+1}) \cdots \hat{a}_{\beta_1}(\tau_{2n}) \rangle. \quad (44)$$

An expectation value of the complex field variables is given as an expectation value of a time ordered product of the creation and annihilation operators in the Heisenberg representation [36]. The time ordering in the imaginary time variable is indicated by the time ordering operator \hat{T} . The ordering begins with the largest imaginary time and ends with the smallest. The rule for a translation of an expectation value of a time ordered product of operators into an expectation value of a product of complex field variables is simply

$$\begin{aligned} & \langle \phi_{\alpha_1}^*(\tau_1) \cdots \phi_{\alpha_n}^*(\tau_n) \phi_{\alpha_{n+1}}(\tau_{n+1}) \cdots \phi_{\alpha_{2n}}(\tau_{2n}) \rangle = \\ & \langle \hat{T} \hat{a}_{\alpha_1}^+(\tau_1) \cdots \hat{a}_{\alpha_n}^+(\tau_n) \hat{a}_{\alpha_{n+1}}(\tau_{n+1}) \cdots \hat{a}_{\alpha_{2n}}(\tau_{2n}) \rangle. \end{aligned} \quad (45)$$

Introducing a time-slice $\varepsilon > 0$, the static n -particle CF (40) can thus be constructed by

$$\begin{aligned} & C_n(\alpha_1, \dots, \alpha_n; \beta_n, \dots, \beta_1) = \\ & \lim_{\varepsilon \rightarrow 0} \langle \hat{a}_{\alpha_1}^+(\tau + (2n-1)\varepsilon) \cdots \hat{a}_{\alpha_n}^+(\tau + n\varepsilon) \hat{a}_{\beta_n}(\tau + (n-1)\varepsilon) \cdots \hat{a}_{\beta_1}(\tau) \rangle = \\ & \lim_{\varepsilon \rightarrow 0} \langle \phi_{\alpha_1}^*(\tau + (2n-1)\varepsilon) \cdots \phi_{\alpha_n}^*(\tau + n\varepsilon) \phi_{\beta_n}(\tau + (n-1)\varepsilon) \cdots \phi_{\beta_1}(\tau) \rangle \end{aligned} \quad (46)$$

Note that this expression is independent of τ . Because the imaginary time is periodic with periodicity $\hbar\beta$, it does not matter which point τ is regarded as the beginning of a period, thus in particular we can assume $\tau = 0$. In general, it is not possible to replace the limit $\varepsilon \rightarrow 0$ simply by putting $\varepsilon = 0$, because the limits for $\varepsilon > 0$ and $\varepsilon < 0$ are not necessarily the same. This feature reflects the fact that the creation and annihilation operators do not commute in the operator formalism.

Some relevant physical quantities which can be calculated from correlation functions shall be mentioned here:

2.2.1 Total particle number

The total particle number is derived from the grand canonical partition function by [3]

$$N_{\text{tot}} = \frac{1}{\beta} \frac{\partial}{\partial \mu} \log Z . \quad (47)$$

Applying Eq. (47) to Z as it is given in Eqs. (32) and (33), we get

$$N_{\text{tot}} = \lim_{\varepsilon \rightarrow 0} \frac{1}{\beta} \frac{1}{Z} \int \left[\sum_{\alpha} \int_0^{\hbar\beta} \phi_{\alpha}^*(\tau + \varepsilon) \phi_{\alpha}(\tau) d\tau \right] e^{-A(\phi^*, \phi)} \mathcal{D}(\phi^*(\tau) \phi(\tau)) .$$

Because of the independence of the CFs of τ , we have

$$N_{\text{tot}} = \lim_{\varepsilon \rightarrow 0} \sum_{\alpha} \langle \phi_{\alpha}^*(\varepsilon) \phi_{\alpha}(0) \rangle . \quad (48)$$

The particle occupation number in state α is

$$n_{\alpha} = \lim_{\varepsilon \rightarrow 0} \langle \phi_{\alpha}^*(\varepsilon) \phi_{\alpha}(0) \rangle . \quad (49)$$

If α denotes a position in space or a lattice site, n_{α} is a local particle density, if α is a momentum index, n_{α} is the momentum distribution of particles.

As has been mentioned before, it is not allowed to put the time-slice $\varepsilon = 0$ in general, because in the discrete-time definition of the action (31), the μ -dependent term is given by

$$-\frac{\beta}{M} \sum_{n=0}^{M-1} \sum_{\alpha} \mu \phi_{\alpha, n+1}^* \phi_{\alpha, n} \quad (50)$$

and therefore occupies the off-diagonal matrix elements in the imaginary time index. It should be noted here, that it is also possible to construct the functional integral with the μ -dependent term being on the diagonal matrix elements, i. e.

$$-\frac{\beta}{M} \sum_{n=0}^{M-1} \sum_{\alpha} \mu \phi_{\alpha, n}^* \phi_{\alpha, n} . \quad (51)$$

In this case the occupation number would be $n_{\alpha} = \langle \phi_{\alpha}^*(0) \phi_{\alpha}(0) \rangle$, which means that the expressions for the physical quantities significantly depend on the definition of the functional integral, which in some cases might be more convenient. However, in this chapter we will keep the off-diagonal representation given in (50).

2.2.2 Condensate density

The condensate density of a BEC is a measure for the off-diagonal long range order of the one-particle CF. It has to do with the spacial range of the one-particle CF and thus α should denote a position vector (in a continuous system) or a lattice site (in an optical lattice). In terms of complex variables, the definition (6) of the condensate density in a system without confining potential is

$$n_0 := \lim_{\mathbf{r} - \mathbf{r}' \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} \langle \phi_{\mathbf{r}}^*(\varepsilon) \phi_{\mathbf{r}'}(0) \rangle . \quad (52)$$

2.2.3 Density-density correlation function

The density-density CF is a two-particle CF. It describes the spacial behaviour of density correlations, which means that here α denotes a position index as well. In terms of field operators it is defined as

$$D(\mathbf{r} - \mathbf{r}') = \langle \hat{n}_{\mathbf{r}} \hat{n}_{\mathbf{r}'} \rangle = \langle \hat{\psi}_{\mathbf{r}}^+ \hat{\psi}_{\mathbf{r}} \hat{\psi}_{\mathbf{r}'}^+ \hat{\psi}_{\mathbf{r}'} \rangle, \quad (53)$$

and in terms of complex field variables it is given as

$$D(\mathbf{r} - \mathbf{r}') = \lim_{\varepsilon \rightarrow 0} \langle \phi_{\mathbf{r}}^*(\varepsilon) \phi_{\mathbf{r}}(0) \phi_{\mathbf{r}'}^*(\varepsilon) \phi_{\mathbf{r}'}(0) \rangle \quad (54)$$

A good physical quantity, which describes correlations of density fluctuations is the truncated density-density CF

$$D_{\text{trunc}}(\mathbf{r} - \mathbf{r}') = \langle \hat{n}_{\mathbf{r}} \hat{n}_{\mathbf{r}'} \rangle - \langle \hat{n}_{\mathbf{r}} \rangle \langle \hat{n}_{\mathbf{r}'} \rangle. \quad (55)$$

The Fourier transform of the density-density CF is called the static structure factor

$$S(\mathbf{q}) = \frac{1}{N_{\text{tot}}} \sum_{\mathbf{r}, \mathbf{r}'} D(\mathbf{r} - \mathbf{r}') e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} . \quad (56)$$

3 Exactly solvable models

3.1 Ideal Bose gas

3.1.1 Hamiltonian and partition function

In this chapter we will survey the basic results of the previously mentioned quantities for an ideal Bose gas. This seems to be reasonable, because it allows us to introduce the methods we will apply for an interacting hard-core Bose gas as well. Contrary to the interacting system, exact analytic results can be found for the non-interacting case of the ideal Bose gas.

A non-interacting Bose gas in a d -dimensional cubic lattice with nearest-neighbour hopping J and lattice constant a is given by the Hamiltonian

$$\hat{H} = J - \frac{J}{2d} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{a}_{\mathbf{r}}^+ \hat{a}_{\mathbf{r}'} + J \sum_{\mathbf{r}} \hat{a}_{\mathbf{r}}^+ \hat{a}_{\mathbf{r}} \quad (57)$$

with the dispersion relation

$$\epsilon_{\mathbf{k}} = J - \frac{J}{d} \sum_{\nu=1}^d \cos(ak_{\nu}), \quad (58)$$

where k_{ν} is the ν -th component of the d -dimensional wave vector \mathbf{k} . Note that the sum over nearest neighbors $\langle \mathbf{r}_i, \mathbf{r}_j \rangle$ means, that the index i runs over the entire lattice and the index j runs over all sites, which are nearest neighbours of j . This means, that each bond appears twice in the sum, once with a hopping process from site i to site j and vice versa. For small wave vectors \mathbf{k} , the lattice dispersion can be approximated by the translation invariant counterpart

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m^*} + \mathcal{O}(\mathbf{k}^4), \quad m^* := \frac{d\hbar^2}{Ja^2}, \quad (59)$$

where m^* is the band mass.

We apply the discrete time action given in Eq. (31) and perform the limit $M \rightarrow \infty$ at the very end. It is possible to write the functional integral (31) in the form

$$Z = \lim_{M \rightarrow \infty} \int \exp \left[- \sum_{\mathbf{k}} \sum_{n,m=1}^M \phi_{\mathbf{k},n}^* \hat{A}_{nm}^{(\mathbf{k})} \phi_{\mathbf{k},m} \right] \prod_{\mathbf{k}} \prod_{n=1}^M d\phi_{\mathbf{k},n}^* d\phi_{\mathbf{k},n} , \quad (60)$$

where the relation between the complex fields in real space and in momentum space is

$$\phi_{\mathbf{r},n} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \phi_{\mathbf{k},n} , \quad (61)$$

and the matrix elements of $\hat{A}^{(\mathbf{k})}$ represent the structure of the discrete imaginary time variable:

$$\hat{A}^{(\mathbf{k})} = \begin{bmatrix} 1 & 0 & \cdots & 0 & -b_{\mathbf{k}} \\ -b_{\mathbf{k}} & 1 & 0 & & \\ 0 & -b_{\mathbf{k}} & 1 & \ddots & \\ & 0 & -b_{\mathbf{k}} & \ddots & 0 \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & \cdots & -b_{\mathbf{k}} & 1 \end{bmatrix} , \quad b_{\mathbf{k}} = 1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} - \mu) . \quad (62)$$

The entry in the upper right corner is necessary to realize the periodic boundary conditions. The Gaussian integral can be integrated out and we get

$$Z = \lim_{M \rightarrow \infty} \prod_{\mathbf{k}} \det \hat{A}^{(\mathbf{k})} = \lim_{M \rightarrow \infty} \prod_{\mathbf{k}} \left[1 - \left(1 - \frac{\beta(\epsilon_{\mathbf{k}} - \mu)}{M} \right)^M \right]^{-1}$$

If we now, as a final step, perform the limit $M \rightarrow \infty$, we get the correct form of the grand canonical partition function of an ideal Bose gas [36]:

$$Z = \prod_{\mathbf{k}} \left[1 - e^{-\beta(\epsilon_{\mathbf{k}} - \mu)} \right]^{-1} . \quad (63)$$

3.1.2 One-particle correlation function

As already discussed in section 2.2, the momentum distribution and the condensate density in a Bose gas can both be described by the one-particle correlation function, cf. Eqs. (48) and (52). Thus we should at first calculate the one-particle CF for an ideal Bose gas in general to determine those quantities. To achieve this we again start with the discrete time functional integral and take the limit $M \rightarrow \infty$ at the end of the calculations. In this sense, we define the imaginary time dependent one-particle CF in momentum space as

$$C(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = \langle \phi_{\mathbf{k}_1, n_1}^* \phi_{\mathbf{k}_2, n_2} \rangle =$$

$$\lim_{M \rightarrow \infty} \frac{1}{Z} \int \phi_{\mathbf{k}_1, n_1}^* \phi_{\mathbf{k}_2, n_2} \exp \left[- \sum_{\mathbf{k}} \sum_{n,m=1}^M \phi_{\mathbf{k},n}^* \hat{A}_{nm}^{(\mathbf{k})} \phi_{\mathbf{k},m} \right] \prod_{\mathbf{k}} \prod_{n=1}^M d\phi_{\mathbf{k},n}^* d\phi_{\mathbf{k},n} , \quad (64)$$

where the indices n_1, n_2 are defined such that

$$\frac{\beta}{M}(n_{1,2} - 1) < \tau_{1,2} < \frac{\beta}{M}n_{1,2} . \quad (65)$$

The Gaussian integral (64) picks out a matrix element of the inverse matrix \hat{A}^{-1} :

$$C(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = \lim_{M \rightarrow \infty} (\hat{A}^{(\mathbf{k}_1)})_{n_2, n_1}^{-1} \delta_{\mathbf{k}_1, \mathbf{k}_2} . \quad (66)$$

Therefore it is necessary to determine the matrix elements of \hat{A}^{-1} . By means of the unitary transformation matrices

$$U_{nm} = \frac{1}{\sqrt{M}} e^{\frac{2\pi i}{M} nm} , \quad U_{nm}^+ = \frac{1}{\sqrt{M}} e^{-\frac{2\pi i}{M} nm} , \quad (67)$$

we can diagonalize the matrix to get

$$(U(\hat{A}^{(\mathbf{k})})^{-1}U^+)_{jn} = \frac{\delta_{jn}}{1 - b_{\mathbf{k}} e^{\frac{2\pi i}{M} n}} ,$$

$$(\hat{A}^{(\mathbf{k})})_{jn}^{-1} = [U^+(U(\hat{A}^{(\mathbf{k})})^{-1}U^+)U]_{jn} = \sum_{l=1}^M \frac{1}{M} \frac{e^{-\frac{2\pi i}{M} l(j-n)}}{1 - b_{\mathbf{k}} e^{\frac{2\pi i}{M} l}} .$$

This sum is given in the Appendix. The result is

$$(\hat{A}^{(\mathbf{k})})_{jn}^{-1} = \frac{1}{1 - b_{\mathbf{k}}^M} \times \begin{cases} b_{\mathbf{k}}^{j-n} & \text{if } j \geq n \\ b_{\mathbf{k}}^{M+n-j} & \text{if } j < n \end{cases} . \quad (68)$$

Performing the limit $M \rightarrow \infty$ in (65) we get

$$C(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = \frac{\delta_{\mathbf{k}_1, \mathbf{k}_2}}{1 - e^{-\beta(\epsilon_{\mathbf{k}} - \mu)}} \times \begin{cases} e^{(\tau_2 - \tau_1)(\epsilon_{\mathbf{k}} - \mu)/\hbar} & \text{if } \tau_1 \geq \tau_2 \\ e^{(\tau_1 - \tau_2 - \hbar\beta)(\epsilon_{\mathbf{k}} - \mu)/\hbar} & \text{if } \tau_1 < \tau_2 \end{cases} . \quad (69)$$

Using this result and the definition (46), the one-particle CF in momentum space for an ideal Bose gas is

$$C_1(\mathbf{k}; \mathbf{k}') = \lim_{\epsilon \rightarrow 0} \langle \phi_{\mathbf{k}}^*(\epsilon) \phi_{\mathbf{k}'}(0) \rangle = \frac{\delta_{\mathbf{k}, \mathbf{k}'}}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} - 1} = \delta_{\mathbf{k}, \mathbf{k}'} N_{\mathbf{k}} , \quad (70)$$

where $n_{\mathbf{k}}$ is the usual momentum distribution of an ideal Bose gas.

In the condensed phase, where the chemical potential takes the value $\mu = 0$, the momentum distribution function diverges at $\mathbf{k} = 0$. In this case, the lowest momentum state $\mathbf{k} = 0$ is macroscopically occupied and builds the condensate. The condensate density in this case is given by

$$n_0 = \frac{N_0}{\mathcal{N}} . \quad (71)$$

The normalisation with the number of lattice sites \mathcal{N} is necessary, because in the BEC phase the ground state is the only macroscopically occupied state, whereas all other occupation numbers are of the order of unity. The total particle density in the condensed phase is the sum of the condensate density and the particle density of all excited states. In the thermodynamic limit, the sum becomes an integral:

$$n_{\text{tot}} = n_0 + \int N_{\mathbf{k}} \frac{d^3 k}{(2\pi)^3} . \quad (72)$$

It should be noted here, that in one and two dimensions a condensate cannot exist. The reason is, that the integral (72) is divergent in these cases if $\mu = 0$, because $n_{\mathbf{k}}$ behaves like k^{-2} for small momenta.

This definition of the condensate density in an ideal Bose gas is also compatible with the more general definition via off-diagonal long range order given in Eq. (52):

$$\lim_{\mathbf{r} - \mathbf{r}' \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle \phi_{\mathbf{r}}^*(\epsilon) \phi_{\mathbf{r}'}(0) \rangle = \lim_{\mathbf{r} - \mathbf{r}' \rightarrow \infty} C(\mathbf{r}; \mathbf{r}') = \lim_{\mathbf{r} - \mathbf{r}' \rightarrow \infty} \int \frac{d^3 k}{(2\pi)^3} N_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')} .$$

3.1.3 Structure factor

From Eqs. (54) and (56) the static structure factor can be obtained. The fourth-order correlation function can be calculated using Wick's theorem (Appendix C):

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \langle \phi_{\mathbf{k}}^*(\varepsilon) \phi_{\mathbf{k}'+\mathbf{q}}^*(0) \phi_{\mathbf{k}+\mathbf{q}}(\varepsilon) \phi_{\mathbf{k}'}(0) \rangle = \\ \lim_{\varepsilon \rightarrow 0} [\langle \phi_{\mathbf{k}}^*(\varepsilon) \phi_{\mathbf{k}+\mathbf{q}}(\varepsilon) \rangle \langle \phi_{\mathbf{k}'+\mathbf{q}}^*(0) \phi_{\mathbf{k}'}(0) \rangle + \langle \phi_{\mathbf{k}}^*(\varepsilon) \phi_{\mathbf{k}'}(0) \rangle \langle \phi_{\mathbf{k}'+\mathbf{q}}^*(0) \phi_{\mathbf{k}+\mathbf{q}}(\varepsilon) \rangle] = \\ N_{\mathbf{k}} \delta_{\mathbf{k}, \mathbf{k}+\mathbf{q}} N_{\mathbf{k}'} \delta_{\mathbf{k}'+\mathbf{q}, \mathbf{k}'} + N_{\mathbf{k}} \delta_{\mathbf{k}, \mathbf{k}'} (N_{\mathbf{k}+\mathbf{q}} + 1) \delta_{\mathbf{k}'+\mathbf{q}, \mathbf{k}+\mathbf{q}}. \end{aligned}$$

For $\mathbf{q} \neq 0$, the first term vanishes. Thus we find the result

$$S(\mathbf{q}) = \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k}} N_{\mathbf{k}} (N_{\mathbf{k}+\mathbf{q}} + 1). \quad (73)$$

In the BEC by separating the ground state and excited states, we get

$$S(\mathbf{q}) = 1 + 2n_0 N_{\mathbf{q}} + \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k} \neq \{0, -\mathbf{q}\}} N_{\mathbf{k}} N_{\mathbf{k}+\mathbf{q}}. \quad (74)$$

Instead of Eq. (54) one can use the more convenient definition in terms of expectation values without time slices

$$S(\mathbf{q}) = 1 + \frac{1}{N_{\text{tot}}} \sum_{\mathbf{k}, \mathbf{k}'} \langle \phi_{\mathbf{k}}^*(0) \phi_{\mathbf{k}'+\mathbf{q}}^*(0) \phi_{\mathbf{k}+\mathbf{q}}(0) \phi_{\mathbf{k}'}(0) \rangle, \quad (75)$$

which leads to Eq. (74) as well. Graphs for different temperature regimes are shown in Fig. 3.

3.1.4 Random walk expansion and world-lines

In this section a very intuitive method of diagrammatically visualizing a grand canonical partition function shall be introduced for an ideal Bose gas in an optical lattice, namely the random walk expansion [38, 39]. We will perform the same expansion in the following chapters for a system of hard-core bosons, in order to demonstrate the effect of the hard-core condition.

The grand canonical partition function of an ideal Bose gas in a d -dimensional cubic lattice is given by the functional integral Eq. (60). But here we use the real-space representation. The time structure of the matrix \hat{A} is the same as in Eq. (62), but instead of the dispersion relation $\epsilon_{\mathbf{k}}$ we use the hopping matrix

$$\hat{J}_{\mathbf{r}\mathbf{r}'} := \begin{cases} -J/2d & \text{if } \mathbf{r}, \mathbf{r}' \text{ nearest neighbours} \\ 0 & \text{otherwise} \end{cases}, \quad (76)$$

which establishes the spacial structure of \hat{A} , and make use of

$$\hat{\epsilon}_{\mathbf{r}\mathbf{r}'} := \hat{J}_{\mathbf{r}\mathbf{r}'} + J \delta_{\mathbf{r}\mathbf{r}'} . \quad (77)$$

Thus we can write

$$\hat{A}_{\mathbf{r}\mathbf{r}'; nm} := \delta_{nm} \delta_{\mathbf{r}\mathbf{r}'} - (\delta_{n, m+1} + \delta_{n1} \delta_{mM}) \left[\delta_{\mathbf{r}\mathbf{r}'} - \frac{\beta}{M} (\hat{\epsilon}_{\mathbf{r}\mathbf{r}'} - \mu \delta_{\mathbf{r}\mathbf{r}'}) \right], \quad (78)$$

where the term $\delta_{n1} \delta_{mM}$ accounts for the upper right matrix element in (62) which arises from the periodicity in imaginary time.

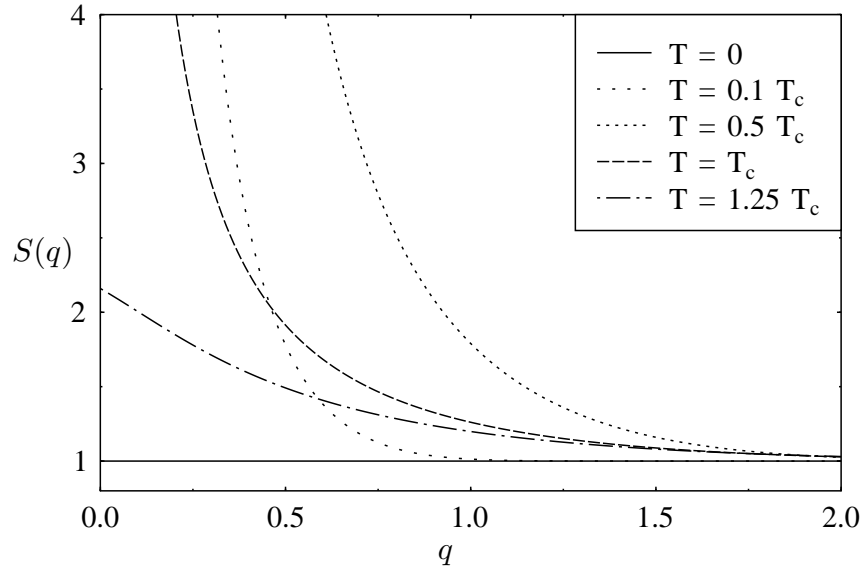


Fig. 3 Static structure factor of an ideal Bose gas of free particles. At $T = 0$, S is constantly unity and has a δ -peak at $q = 0$. At $0 < T < T_c$ it diverges, and at $T > T_c$ it reaches a constant near $q = 0$. All cases are characterised by the relation $\lim_{q \rightarrow \infty} S(q) = 1$.

The idea of the random walk expansion is to expand the off-diagonal part of the exponential in the functional integral expression in terms of the field variables:

$$\exp \left[- \sum_{\mathbf{r}, \mathbf{r}'} \sum_{n,m=1}^M \phi_{\mathbf{r},n}^* \hat{A}_{\mathbf{r}\mathbf{r}';nm} \phi_{\mathbf{r}',m} \right] =$$

$$\exp \left[- \sum_{\mathbf{r}} \sum_{n=1}^M \phi_{\mathbf{r},n}^* \phi_{\mathbf{r},n} \right] \sum_{\{l_{\mathbf{r}\mathbf{r}'} \geq 0\}} \frac{1}{l_{\mathbf{r}\mathbf{r}'}!} \left[\prod_{\mathbf{r}, \mathbf{r}', n} \phi_{\mathbf{r},n}^* \underbrace{\left(\delta_{\mathbf{r}\mathbf{r}'} - \frac{\beta}{M} (\hat{\epsilon}_{\mathbf{r}\mathbf{r}'} - \mu \delta_{\mathbf{r}\mathbf{r}'}) \right)}_{=:\hat{u}_{\mathbf{r}\mathbf{r}'}} \phi_{\mathbf{r}',n-1} \right]^{l_{\mathbf{r}\mathbf{r}',n}}$$

The abbreviation $\hat{u}_{\mathbf{r}\mathbf{r}'}$ has been introduced for convenience. The functional integral can be solved by using the identities

$$\prod_{\mathbf{r}, \mathbf{r}', n} (\phi_{\mathbf{r},n}^* \phi_{\mathbf{r}',n-1})^{l_{\mathbf{r}\mathbf{r}',n}} = \prod_{\mathbf{r}, n} [(\phi_{\mathbf{r},n}^*)^{m_{\mathbf{r},n}} (\phi_{\mathbf{r},n})^{m'_{\mathbf{r},n}}] , \quad (79)$$

$$\text{where } m_{\mathbf{r},n} := \sum_{\mathbf{r}'} l_{\mathbf{r}\mathbf{r}',n} \text{ and } m'_{\mathbf{r},n} := \sum_{\mathbf{r}'} l_{\mathbf{r}'\mathbf{r},n+1}$$

and

$$\int (\phi^*)^m \phi^{m'} e^{-\phi^* \phi} \frac{d\phi^* d\phi}{2\pi i} = m! \delta_{mm'} . \quad (80)$$

This results in the following form of the grand canonical partition function as a sum over all indices $l_{\mathbf{r}\mathbf{r}',n}$:

$$Z = \sum_{\{l_{\mathbf{r}\mathbf{r}',n} \geq 0\}} \prod_{\mathbf{r}, n} (m_{\mathbf{r},n}! \delta_{m_{\mathbf{r},n}, m'_{\mathbf{r},n}}) \prod_{\mathbf{r}, \mathbf{r}', n} \left[\frac{(\hat{u}_{\mathbf{r}\mathbf{r}'})^{l_{\mathbf{r}\mathbf{r}',n}}}{l_{\mathbf{r}\mathbf{r}',n}!} \right] . \quad (81)$$

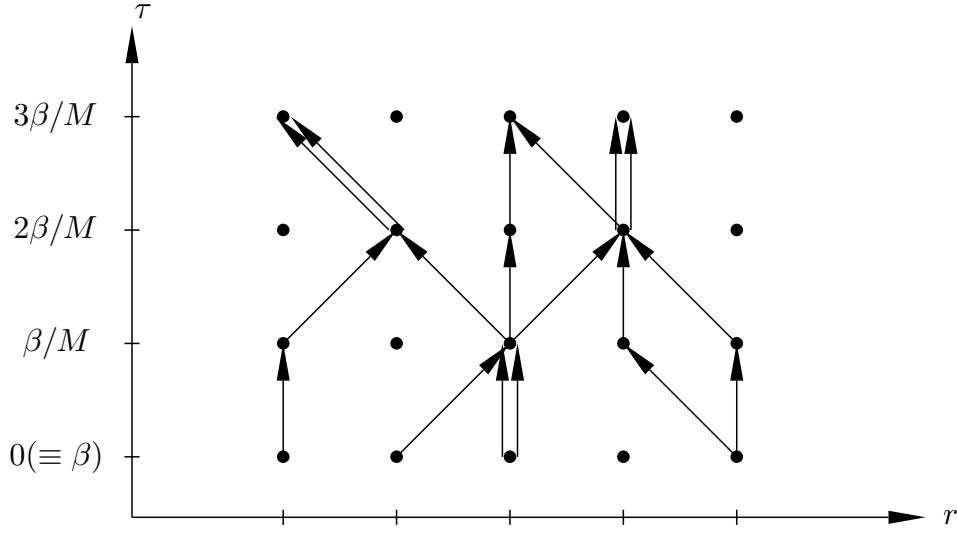


Fig. 4 Random walk expansion of an ideal Bose gas; world-line diagram.

Note that it is necessary to define $(\hat{u}_{\mathbf{r}\mathbf{r}'})^0 \equiv 1$ here, even for the vanishing matrix elements of \hat{u} .

One possible interpretation of this expression is as follows: Each term of the sum can be represented by a diagram, where a particle propagation from site \mathbf{r} at imaginary time τ to site \mathbf{r}' at time $\tau + \hbar\beta/M$ is indicated by an arrow. So each particle is characterised by a “world-line” showing its movement through the lattice in imaginary time. The contribution of a certain diagram is defined by the following properties:

- The number of particles (arrows) propagated from site \mathbf{r}' at time $(n - 1)\hbar\beta/M$ to site \mathbf{r} at time $n\hbar\beta/M$ is given by $l_{\mathbf{r}\mathbf{r}',n}$. In the case of nearest neighbour hopping, particle propagation in one time step $\hbar\beta/M$ is only possible between neighbouring sites, or the particle stays at the same site.
- The number of particles (arrows) which are propagated to site \mathbf{r} at time $n\hbar\beta/M$ from the previous time step is $m_{\mathbf{r},n}$.
- The number of particles (arrows) propagating from site \mathbf{r} at time $n\hbar\beta/M$ to the next time step is $m'_{\mathbf{r},n}$.
- Particle conservation is assured by the δ -function in Eq. (81), such that $m_{\mathbf{r},n} = m'_{\mathbf{r},n}$ is equal to the number of particles at site \mathbf{r} and time $n\hbar\beta/M$.
- There is a periodicity in imaginary time: Time $\tau = \hbar\beta$ is equivalent to time $\tau = 0$, so the diagrams have to be periodic in time.

Note that in the ideal Bose gas $m_{\mathbf{r},n} > 1$ is possible, i.e. more than one particle can occupy the same lattice site at the same time. This will be excluded to establish the hard-core interaction in a Bose gas.

3.2 Hard-core bosons in 1D

3.2.1 General remarks

The main feature of the one-dimensional hard-core Bose gas is, that the particles cannot interchange their position. An interesting consequence of this property is the equivalence to an ideal non-interacting one-dimensional Fermi gas. However, it is important to mention, that this equivalence does not hold for all

physical quantities in momentum space, namely for those which are given by one-particle correlation functions like the momentum distribution [40, 41, 42, 43, 44]. It is possible to calculate the momentum distribution by means of a Jordan-Wigner transformation (see e. g. refs. [36, 45]). This approach has been used in a couple of works [28, 46, 47]. However, this problem will not be addressed here. On the other hand, quantities given by two-particle correlation functions like the density-density correlation function and the dynamic structure factor are the same for hard-core bosons and for ideal fermions.

The zero temperature phase diagram of a hard-core Bose gas in a one-dimensional optical lattice shows three phases [48]: An empty phase (EP), an incommensurate phase (ICP) with a particle number per lattice site of $0 < n_{\text{tot}} < 1$, and a Mott insulator (MI) with $n_{\text{tot}} = 1$. Here we will especially be interested in the phase transition between the ICP and the MI phase for zero and non-zero temperatures. Again, the quantity we chose for investigating this transition is the static structure factor. It has also been considered in other works about one-dimensional Bose gases, in the weakly interacting regime as well as in the strongly interacting regime [49, 50, 51, 52].

As has been demonstrated for the ideal Bose gas, a random walk expansion leads to a world-line picture. To make the mapping to a system of ideal fermions possible, it has to be assured that world lines cannot intersect each other. So instead of constructing the functional integral by starting from the Hamiltonian, we choose a different way and construct it by starting out from the random-walk picture directly.

When the random walk expansion for a system of ideal spinless fermions is performed, one obtains a sum which is analogous to the sum in Eq. (81) with two important differences: Because of the nilpotent property of the Grassmann variables, the fermionic analog to Eq. (80) reads

$$\int \bar{\psi}^m \psi^{m'} e^{-\bar{\psi}\psi} d\psi d\bar{\psi} = \delta_{mm'} (\delta_{m,0} + \delta_{m,1}) . \quad (82)$$

This means that all terms, where the particle number $m_{r,n}$ or $m'_{r,n}$ is larger than 1 at lattice site r , do not contribute. This reflects the Pauli principle or in the case of hard-core bosons, the hard-core property. The second is that the Grassmann variable analog to Eq. (79) gets an additional sign because of the anti-commutation property. To avoid this problem it is possible to construct a world-line model where world-lines do not intersect. For this purpose we adopt an approach to the statistics of directed polymers in two dimensions [53].

3.2.2 Particle density and phase diagram

It has been shown that the grand canonical partition function is given by the functional integral [48]

$$Z = \lim_{M \rightarrow \infty} \int \exp \left[- \sum_k \sum_{n=1}^M \sum_{j,j'=1}^2 \bar{\psi}_{k,n,j} \frac{[\hat{G}_n^{-1}(k)]_{jj'}}{1 - \frac{\beta}{M}\mu} \psi_{k,n,j'} \right] \prod_{k,n,j} d\psi_{k,n,j} d\bar{\psi}_{k,n,j} \quad (83)$$

with the 2×2 matrix

$$\hat{G}_n^{-1}(k) = \begin{pmatrix} -e^{\frac{2\pi i}{M}(n-\frac{1}{2})} + 1 - \frac{\beta}{M}\mu & -\frac{\beta}{M}\frac{J}{2}e^{\frac{2\pi i}{M}(n-\frac{1}{2})}(1 + e^{ik}) \\ -\frac{\beta}{M}\frac{J}{2}(1 + e^{-ik}) & -e^{\frac{2\pi i}{M}(n-\frac{1}{2})} + 1 - \frac{\beta}{M}\mu \end{pmatrix} . \quad (84)$$

This integral can be performed and it yields

$$Z = \lim_{M \rightarrow \infty} \left(1 - \frac{\beta}{M}\mu \right)^{-2MN} \det \hat{G}^{-1} , \quad (85)$$

where \mathcal{N} is the number of lattice sites. The one-particle correlation function of the fermions at equal times can be calculated as

$$C(k) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{n,m=1}^M \hat{G}_{11}(k)_{nm} \quad (86)$$

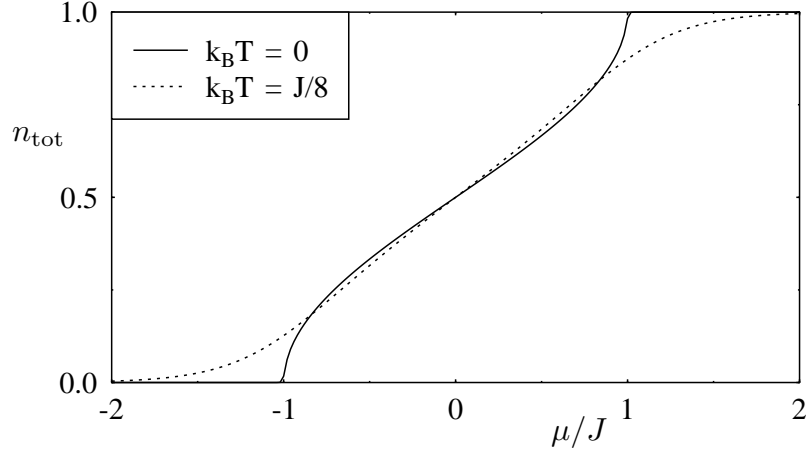


Fig. 5 Total particle density of a hard-core Bose gas in a one-dimensional optical lattice calculated from Eq. (89), for both zero temperature (solid line) and finite temperature (dashed line).

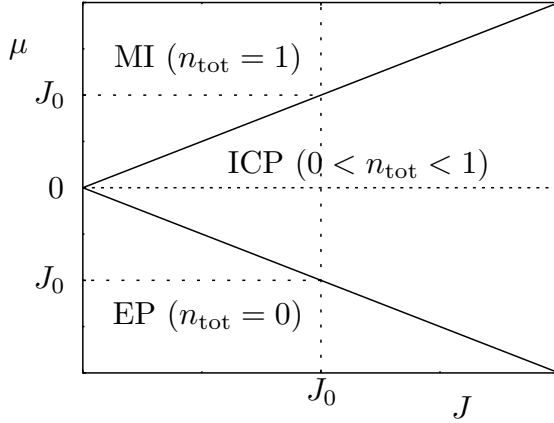


Fig. 6 Phase diagram of the one-dimensional hard-core Bose gas at zero temperature with an empty phase (EP), an incommensurate phase (ICP), and a Mott insulator (MI).

This sum is performed in Appendix A.4. After performing the limit $M \rightarrow \infty$, the result is

$$C(k) = \frac{1}{2} \left(\frac{1}{1 + e^{-\beta(J \cos \frac{k}{2} - \mu)}} + \frac{1}{1 + e^{-\beta(-J \cos \frac{k}{2} - \mu)}} \right). \quad (87)$$

As was mentioned before, the one-particle correlation function does not lead to the momentum distribution. However, the total particle density of the bosons is given by taking the fermionic one-particle correlation function in real space

$$C(r, r') = \int_0^{2\pi} C(k) e^{ik(r-r')} \frac{dk}{2\pi} \quad (88)$$

at $r = r'$. This can be shown by applying the expression (47) of the total particle number to the partition function (83). We need an additional factor of $1/2$ because of our special construction:

$$\begin{aligned} N_{\text{tot}} &= \frac{1}{2\beta} \frac{\partial}{\partial \mu} \log Z = \lim_{M \rightarrow \infty} \frac{1}{2\beta} \frac{\partial}{\partial \mu} \left[-2M\mathcal{N} \log \left(1 - \frac{\beta}{M} \mu \right) - \log \det \hat{G} \right] \\ &= \mathcal{N} - \frac{1}{2\beta Z} \lim_{M \rightarrow \infty} \frac{\beta}{M} \sum_{r,n,j} \langle \bar{\psi}_{r,t,j} \psi_{r,t,j} \rangle \end{aligned}$$

So, because of $\langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \rangle = \langle \bar{\psi}_{r,n,2} \psi_{r,n,2} \rangle = C(r, r)$, we find the result

$$n_{\text{tot}} = \frac{N_{\text{tot}}}{\mathcal{N}} = 1 - C(r, r) \quad (89)$$

for the total particle density. Note that the time slice ε , which was necessary for the definition of the total particle density for weakly interacting bosons (see Eq. (48)), is absent here, because of the construction of the Green's matrix. The zero temperature result is

$$\lim_{\beta \rightarrow \infty} n_{\text{tot}} = \begin{cases} 0 & \text{if } \mu < -J \\ 1 - \frac{1}{\pi} \arccos \left(\frac{\mu}{J} \right) & \text{if } -J < \mu < J \\ 1 & \text{if } \mu > J \end{cases} \quad (90)$$

Graphs for zero temperature and finite temperature are plotted in Fig. 5. Both graphs are symmetric to the point $\mu/J = 0$, $n_{\text{tot}} = 1/2$. This reflects the particle hole symmetry of the system: Because of the Pauli principle a given configuration of the system is symmetric to the configuration, in which each occupied site is empty and vice versa. Further one can see that the system is empty ($n_{\text{tot}} = 0$) if $\mu/J < -1$, and it is a Mott-insulator ($n_{\text{tot}} = 1$) if $\mu/J > 1$. The phase transitions between the EP and the incommensurate phase with $0 < n_{\text{tot}} < 1$, and between the ICP and the MI, are characterised by a diverging slope of the curve at the transition points. At non-zero temperatures the sharp phase transition is smeared out. The zero temperature phase diagram is depicted schematically in Fig. 6.

3.2.3 Density correlations and static structure factor

We define the truncated density-density CF of the hard-core Bose gas as

$$D(r - r') = \langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \bar{\psi}_{r',n,1} \psi_{r',n,1} \rangle - \underbrace{\langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \rangle \langle \bar{\psi}_{r',n,1} \psi_{r',n,1} \rangle}_{= n_{\text{tot}}^2} \quad (91)$$

Using Wick's theorem for Grassmann variables as given in Appendix C, we find

$$\langle \bar{\psi}_{r,n,1} \psi_{r,n,1} \bar{\psi}_{r',n,1} \psi_{r',n,1} \rangle = n_{\text{tot}}^2 - C(r, r') C(r', r),$$

leading to the result

$$D(r - r') = -C(r, r') C(r', r). \quad (92)$$

The static structure factor is related to the density-density CF by means of a Fourier transformation which is shifted by unity, and a normalisation. We use the definition [48, 50]

$$S(q) = 1 + \frac{\sum_{r,r'} D(r - r') e^{iq(r-r')}}{\sum_{r,r'} D(r - r')}. \quad (93)$$

It is the analog to the definition of the static structure factor of an ideal Bose gas (75), where the term 1 appears when the time slice is canceled in the expectation value of the complex fields. Expressed in terms

of the one-particle CF in momentum space $C(k)$ by applying the Fourier transformation in Eq. (88), the above expression reads

$$S(q) = 1 - \frac{\int_0^{2\pi} C(k)C(k+q) dk}{\int_0^{2\pi} C(k)^2 dk}. \quad (94)$$

We want to investigate the static structure factor at zero temperature in the ICP near the phase transitions to the EP and the MI. Because of the particle-hole symmetry discussed in the previous section, both transitions should be symmetric with respect to the physics of light scattering. Let us first discuss the region $\mu > 0$. Defining the characteristic wave vector k^* we find the result

$$S(q) = \begin{cases} \frac{q}{2k^*} & \text{if } q < 2k^* \\ 1 & \text{if } 2k^* < q < 2\pi - 2k^* \\ \frac{2\pi - q}{2k^*} & \text{if } q > 2\pi - 2k^* \end{cases}. \quad (95)$$

In order to keep the particle hole symmetry for the static structure factor, in the region $\mu < 0$ we make the substitution $C(k) \rightarrow 1 - C(k)$ in the expression (94), and find the same result as in Eq. (95). The expression for the density-density CF $D(r - r')$ near both phase transitions we get from the Eqs. (88) and (92). At zero temperature it is

$$D(r - r') = \left(\frac{\sin(k^*(r - r'))}{2\pi(r - r')} \right)^2. \quad (96)$$

The characteristic wave vector can be written in terms of the total particle density (89):

$$k^* = \begin{cases} 2\pi n_{\text{tot}} & \text{if } n_{\text{tot}} < 1/2 \\ 2\pi(1 - n_{\text{tot}}) & \text{if } n_{\text{tot}} > 1/2 \end{cases}. \quad (97)$$

Near the phase transitions where $\delta := |\mu - \mu_c|/J \ll 1$, we have $\mu = (1 - \delta)J$ at the ICP-MI phase transition, and $\mu = -(1 - \delta)J$ at the ICP-EP transition. Here, we can approximate

$$k^* \approx \sqrt{8\delta}. \quad (98)$$

For a homogeneous impenetrable Bose gas the role of k^* is played by the Fermi wave vector $k_F = \pi n_{\text{tot}}$ [50]. In our result (97), k^* depends linearly on the density as well as in the region $n_{\text{tot}} < 1/2$, but the discontinuous slope of the function $k^*(n_{\text{tot}})$ at the point $n_{\text{tot}} = 1/2$ is a consequence of the optical lattice potential. The relation (23) allows us to identify the excitation spectrum

$$\epsilon(q) = \hbar c q + \mathcal{O}(q^2), \quad c = \frac{\hbar k^*}{m}. \quad (99)$$

which is linear for small values of q , where c is the sound velocity. The density-density CF and the static structure factor near the ICP-MI phase transition are plotted in Fig. 7.

The density-density CF shows characteristic oscillations with length $\lambda = \pi/k^*$. This length scale diverges at the ICP-EP and ICP-MI phase transition with $1/n_{\text{tot}}$ and $1/(1 - n_{\text{tot}})$, respectively. Thus it can be used as a measure for the distance of the system to one of the two phase transitions. In the EP and the MI phase, the density-density CF vanishes because of the absence of particle number fluctuations, and the static structure factor saturates to $S(q) \equiv 1$.

3.2.4 External trap potential

In the previous sections a system in a translational invariant lattice was considered. Calculations have also been made for a one-dimensional Bose gas in a harmonic trap potential [48]

$$V(r) = \frac{m}{2} \omega_{\text{ho}}^2 (ar)^2, \quad (100)$$

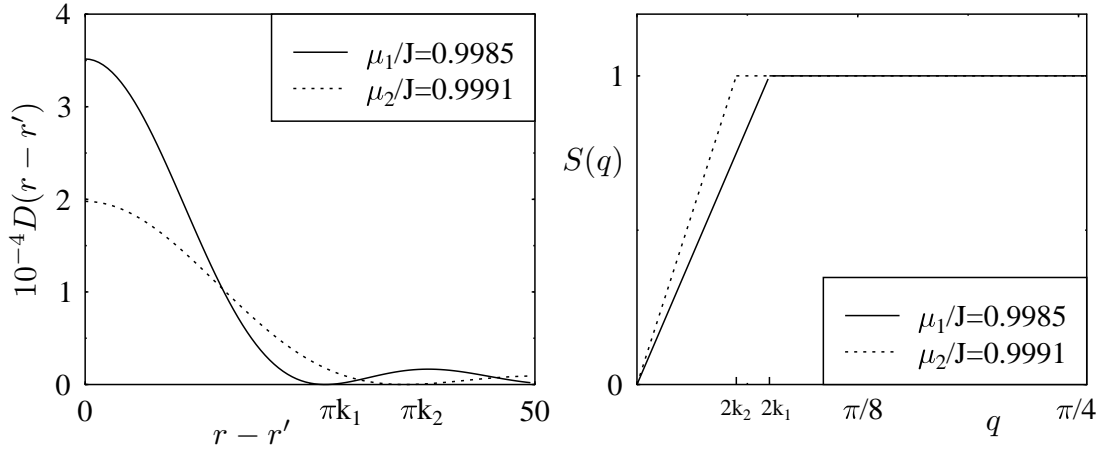


Fig. 7 Truncated density-density correlation function $D(r-r')$ and static structure factor $S(q)$ in the vicinity of the ICP-MI phase transition. The transition point is at $\mu_c = J$. For the ICP-EP phase transition, the situation is symmetrical.

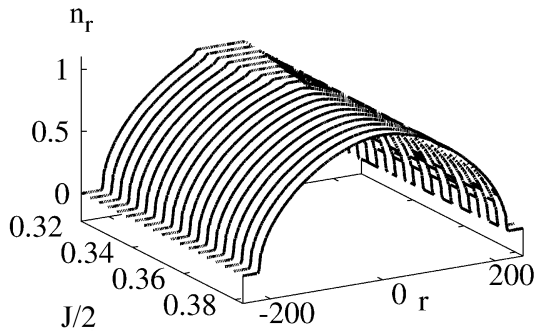


Fig. 8 Local particle density for system in harmonic trap potential ($\mu = 0.7$, $ma^2\omega_{\text{ho}}^2/2 = 3 \times 10^{-5}$) with varying tunneling rate J . A Mott plateau appears in the center of the trap ($r=0$) as J is decreased below a critical value $J_P \approx 0.70$. (Fig. taken from ref. [48].)

where again a is the lattice constant, and ω_{ho} is the harmonic oscillator frequency of the trap. The numerical result for the local particle density at zero temperature is plotted in Fig. 8, where the formation of a Mott plateau can be seen below a critical value J_P . A similar behavior was found for the one-dimensional Bose-Hubbard model with a harmonic trapping potential [54].

The properties of the density-density CF and the static structure factor are qualitatively the same as in the translational invariant case. $D(r)$ vanishes when J_P is reached, owing to the fact that there are no density fluctuations within the plateau. The characteristic length scales become larger as the Mott plateau is reached.

4 Weakly interacting bosons: Bogoliubov theory

Before discussing an interacting Bose gas in an optical lattice, we begin with the derivation of the Bogoliubov approximation for a dilute homogeneous Bose gas. Although the Bogoliubov theory can also be applied for bosons in a lattice potential, a Mott-insulating phase is not found within this approximation [55]. Many aspects of the physics discussed in this chapter show up in the hard-core Bose gases in optical lattices as well.

4.1 Derivation from saddle point approximation

It might be interesting to derive the results of Bogoliubov theory from the functional integral point of view. The method which will be used here and in the following chapters is the saddle point approximation (or: stationary phase approximation, Gaussian approximation) [36, 56, 57]. It allows to find a mean-field solution plus fluctuations around the mean-field result. The mean-field solution is connected to the condensate order parameter, while the fluctuations contain the information about the quasiparticles and their spectrum. The saddle-point approximation is good as long as these fluctuations are small.

The main idea of a saddle point approximation is to expand the action of the system around its minimum up to second order in the field variables. This leads to a Gaussian integral which can be performed. The action of a bosonic system is given in Eq. (33), where in this case the index α shall denote the position vector \mathbf{r} . Together with the Hamiltonian (5) of the interacting Bose gas we have

$$A(\phi^*, \phi) = \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \int d^3r \left\{ \phi^*(\mathbf{r}, \tau) \left[\left(\hbar \frac{\partial}{\partial \tau} - \mu \right) - \frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \phi(\mathbf{r}, \tau) + \frac{g}{2} |\phi(\mathbf{r}, \tau)|^4 \right\}. \quad (101)$$

By minimising A with respect to the complex fields we get a mean-field equation for the condensate order parameter $\Phi_0(\mathbf{r}, \tau)$:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g |\Phi_0(\mathbf{r}, \tau)|^2 \right) \Phi_0(\mathbf{r}, \tau) = - \left(\frac{\partial}{\partial \tau} - \mu \right) \Phi_0(\mathbf{r}, \tau). \quad (102)$$

After performing the analytic continuation $\frac{\partial}{\partial \tau} \rightarrow -i\hbar \frac{\partial}{\partial t}$ and omitting the chemical potential term, this is identical to the time-dependent Gross-Pitaevskii equation (12). We recall that the invariance of the mean-field solution under a gauge transformation (9) with global phase α reflects the broken global $U(1)$ symmetry of the BEC phase.

To find the results from the previous sections in this chapter, we assume a homogeneous system, i.e. $V_{\text{ext}}(\mathbf{r}) \equiv 0$ in the action (101). Further we assume that the mean-field solution is constant in space and imaginary time: $\Phi_0(\mathbf{r}, \tau) \equiv \Phi_0$. In this case, the solution of Eq. (102) is

$$|\Phi_0|^2 = n_0 = \frac{\mu}{g}. \quad (103)$$

We now write the complex field as the sum of the mean-field solution plus fluctuations

$$\phi(\mathbf{r}, \tau) = \Phi_0 + \delta\phi(\mathbf{r}, \tau), \quad \phi^*(\mathbf{r}, \tau) = \Phi_0^* + \delta\phi^*(\mathbf{r}, \tau), \quad (104)$$

where the complex field of fluctuations $\delta\phi$ is considered to be small, such that those terms in the action which are of higher than second order in the fluctuations, can be neglected. We split the quasiparticle field

into its real and imaginary part and write $\delta\phi(\mathbf{r}, \tau) = \delta\phi' + i\delta\phi''$, $\delta\phi^*(\mathbf{r}, \tau) = \delta\phi' - i\delta\phi''$. The expansion yields

$$A \approx A_0 + \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \int d^3r \begin{pmatrix} \delta\phi' \\ \delta\phi'' \end{pmatrix} \cdot \begin{pmatrix} -\frac{\hbar^2}{2m} \nabla^2 & -i\hbar \frac{\partial}{\partial \tau} \\ i\hbar \frac{\partial}{\partial \tau} & -\frac{\hbar^2}{2m} \nabla^2 + 2\mu \end{pmatrix} \begin{pmatrix} \delta\phi' \\ \delta\phi'' \end{pmatrix}, \quad (105)$$

where we have already eliminated the condensate order parameter by Eq. (103), and the zeroth-order part of the action is

$$A_0 = \beta V \left(-\mu |\Phi_0|^2 + \frac{g}{2} |\Phi_0|^4 \right) = -\frac{\beta V \mu^2}{2g}. \quad (106)$$

Because A_0 does not depend on the field fluctuations, and the second term is of second order in $\delta\phi$ and $\delta\phi^*$, the functional integral for the grand canonical partition function

$$Z = \int e^{-A(\delta\phi', \delta\phi'')} \mathcal{D}(\delta\phi'(\mathbf{r}, \tau) \delta\phi''(\mathbf{r}, \tau)) \quad (107)$$

can be performed because it is Gaussian. We Fourier transform the field of fluctuations with respect to the spacial coordinate like

$$\delta\phi'(\mathbf{r}, \tau) = \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{k}} \delta\phi'_{\mathbf{k}}(\tau) \cos(\mathbf{k} \cdot \mathbf{r}) \quad (108)$$

$$\delta\phi''(\mathbf{r}, \tau) = \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{k}} \delta\phi''_{\mathbf{k}}(\tau) \cos(\mathbf{k} \cdot \mathbf{r}), \quad (109)$$

with the constraints $\delta\phi'_{\mathbf{k}} = \delta\phi'_{-\mathbf{k}}$ and $\delta\phi''_{\mathbf{k}} = \delta\phi''_{-\mathbf{k}}$ and thus get

$$A = A_0 + \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \sum_{\mathbf{k}} \begin{pmatrix} \delta\phi'_{\mathbf{k}}(\tau) \\ \delta\phi''_{\mathbf{k}}(\tau) \end{pmatrix} \cdot \begin{pmatrix} \epsilon_{\mathbf{k}} & -i\hbar \frac{\partial}{\partial \tau} \\ i\hbar \frac{\partial}{\partial \tau} & \epsilon_{\mathbf{k}} + 2\mu \end{pmatrix} \begin{pmatrix} \delta\phi'_{\mathbf{k}}(\tau) \\ \delta\phi''_{\mathbf{k}}(\tau) \end{pmatrix} \quad (110)$$

with the free-particle dispersion relation $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$. It is further possible to perform a Fourier transformation with respect to the imaginary time coordinate as well, namely

$$\delta\phi'_{\mathbf{k}}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \delta\phi'_{\mathbf{k}, \omega_n} \cos(\omega_n \tau) \quad (111)$$

$$\delta\phi''_{\mathbf{k}}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \delta\phi''_{\mathbf{k}, \omega_n} \cos(\omega_n \tau), \quad (112)$$

with the Matsubara frequencies for bosons $\omega_n = 2\pi n / \hbar\beta$ and the constraints $\delta\phi'_{\mathbf{k}, \omega_n} = \delta\phi'_{\mathbf{k}, -\omega_n}$ and $\delta\phi''_{\mathbf{k}, \omega_n} = \delta\phi''_{\mathbf{k}, -\omega_n}$. This leads to the form

$$A = A_0 + \sum_{\mathbf{k}, n} \begin{pmatrix} \delta\phi'_{\mathbf{k}, \omega_n} \\ \delta\phi''_{\mathbf{k}, \omega_n} \end{pmatrix} \cdot \mathcal{G}^{-1}(\mathbf{k}, \omega_n) \begin{pmatrix} \delta\phi'_{\mathbf{k}, \omega_n} \\ \delta\phi''_{\mathbf{k}, \omega_n} \end{pmatrix}, \quad (113)$$

and allows to identify the quasiparticle Green's function (a 2×2 matrix in this case)

$$\mathcal{G}^{-1}(\mathbf{k}, i\hbar\omega_n) = \begin{pmatrix} \epsilon_{\mathbf{k}} & i\hbar\omega_n \\ i\hbar\omega_n & \epsilon_{\mathbf{k}} + 2\mu \end{pmatrix}. \quad (114)$$

The excitation energies of the quasiparticles are given by the poles of the quasiparticle Green's function [36], which are found by solving the equation

$$\det \mathcal{G}^{-1}(\mathbf{k}, i\hbar\omega_n) = 0. \quad (115)$$

After performing the analytic continuation $i\hbar\omega_n \longrightarrow E_{\mathbf{k}}$ we get

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}(2\mu + \epsilon_{\mathbf{k}})}, \quad (116)$$

which is identical to the Bogoliubov spectrum, if the relation $n_0 = \mu/g$ is inserted.

4.2 Partition function and condensate depletion

To find the correct expression for the grand canonical partition function as well as for the correlation functions, we have to perform the same steps as in section 3.1.1, namely to start with the discrete-time functional integral and sending the number of time steps M to infinity at the end. By analogy with Eq. (60), the discrete-time version of Eq. (110) is

$$A_{\text{discrete}} = A_0 + \sum_{\mathbf{k}} \sum_{n,m=1}^M \begin{pmatrix} \delta\phi'_{\mathbf{k},n} \\ \delta\phi''_{\mathbf{k},n} \end{pmatrix} \cdot \hat{A}_{nm}^{(\mathbf{k})} \begin{pmatrix} \delta\phi''_{\mathbf{k},m} \\ \delta\phi'_{\mathbf{k},m} \end{pmatrix}, \quad (117)$$

where $\hat{A}_{nm}^{(\mathbf{k})}$ has the $M \times M$ structure

$$\hat{A}^{(\mathbf{k})} = \begin{bmatrix} \hat{B} & -\hat{b}_{\mathbf{k}}^* & 0 & \cdots & 0 & -\hat{b}_{\mathbf{k}} \\ -\hat{b}_{\mathbf{k}} & \hat{B} & -\hat{b}_{\mathbf{k}}^* & 0 & & \\ 0 & -\hat{b}_{\mathbf{k}} & \hat{B} & \ddots & & \vdots \\ & 0 & -\hat{b}_{\mathbf{k}} & \ddots & -\hat{b}_{\mathbf{k}}^* & 0 \\ \vdots & & 0 & \ddots & \hat{B} & -\hat{b}_{\mathbf{k}}^* \\ -\hat{b}_{\mathbf{k}}^* & & & \cdots & -\hat{b}_{\mathbf{k}} & \hat{B} \end{bmatrix} \quad (118)$$

in the imaginary time variables n and m , and each matrix entry is by itself a 2×2 matrix:

$$\hat{b}_{\mathbf{k}} = \frac{1}{2} \left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} + \mu) \right) \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 1 + \frac{\beta}{M}\mu & 0 \\ 0 & 1 - \frac{\beta}{M}\mu \end{pmatrix}. \quad (119)$$

The matrix can be diagonalized by using the same unitary transformation (67), which was applied for the ideal Bose gas. This yields

$$(U \hat{A}^{(\mathbf{k})} U^+)_{kn} = \delta_{kn} \left[\begin{pmatrix} 1 + \frac{\beta}{M}\mu & 0 \\ 0 & 1 - \frac{\beta}{M}\mu \end{pmatrix} - \left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} + \mu) \right) \begin{pmatrix} \cos\left(\frac{2\pi}{M}n\right) & \sin\left(\frac{2\pi}{M}n\right) \\ -\sin\left(\frac{2\pi}{M}n\right) & \cos\left(\frac{2\pi}{M}n\right) \end{pmatrix} \right]. \quad (120)$$

Using the product given in Appendix A.6, the determinant of the matrix can be found as

$$\det \hat{A}^{(\mathbf{k})} = \left(1 - \frac{\beta}{M}(\epsilon_{\mathbf{k}} + \mu) \right) \left[-2 + \left(1 + \frac{\beta}{M} \sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2\mu)} + \mathcal{O}\left(\frac{\beta}{M}\right)^2 \right)^M + \left(1 - \frac{\beta}{M} \sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2\mu)} + \mathcal{O}\left(\frac{\beta}{M}\right)^2 \right)^M \right]. \quad (121)$$

Thus we obtain the grand canonical partition function of the Bogoliubov Hamiltonian (after omitting a constant factor):

$$Z = e^{-A_0} \lim_{M \rightarrow \infty} \prod_{\mathbf{k} \neq 0} [\det \hat{A}^{(\mathbf{k})}]^{-\frac{1}{2}} = \exp\left(\frac{\beta V \mu^2}{2g}\right) \prod_{\mathbf{k} \neq 0} e^{\frac{\beta}{2}(\epsilon_{\mathbf{k}} + \mu)} [\cosh(\beta E_{\mathbf{k}}) - 1]^{-\frac{1}{2}}. \quad (122)$$

The distribution function of the particles outside of the condensate is given as

$$\langle n_{\mathbf{k}} \rangle = \langle \delta \phi_{\mathbf{k}}^*(0) \delta \phi_{\mathbf{k}}(0) \rangle = \langle \delta \phi_{\mathbf{k}}'(0)^2 \rangle + \langle \delta \phi_{\mathbf{k}}''(0)^2 \rangle = \lim_{M \rightarrow \infty} \frac{1}{2} \left(([\hat{A}^{(\mathbf{k})}]_{11}^{-1})_{nn} + ([\hat{A}^{(\mathbf{k})}]_{22}^{-1})_{nn} \right), \quad (123)$$

with the 11- and the 22-component of the matrix with respect to the 2×2 structure. After inversion of the matrix (120) and the back transformation, the matrix elements can be found and after performing the limit $M \rightarrow \infty$ we get

$$\langle n_{\mathbf{k}} \rangle = -\frac{1}{2} + \frac{\epsilon_{\mathbf{k}} + \mu}{2E_{\mathbf{k}}} \coth \left(\frac{\beta}{2} E_{\mathbf{k}} \right). \quad (124)$$

The quantity

$$n_{\text{tot}} - n_0 = \int \langle n_{\mathbf{k}} \rangle \frac{d^3 k}{(2\pi)^3} \quad (125)$$

is called condensate depletion. Contrary to the ideal Bose gas it is non-zero at zero temperature.

4.3 Static structure factor

The static structure factor is given by the fourth-order expectation value (75), which we used for the ideal gas before. We replace ϕ_0 by the order parameter Φ_0 and for non-zero momenta we replace $\phi_{\mathbf{k}} \rightarrow \delta \phi_{\mathbf{k}}$. After splitting the fluctuations into real and imaginary part and applying Wick's theorem for real variables, we get a similar result as in Eq. (74). The difference to the ideal Bose gas is, that the anomalous expectation values $\langle \phi_{\mathbf{k}}^* \phi_{-\mathbf{k}} \rangle$ and $\langle \phi_{\mathbf{k}} \phi_{-\mathbf{k}} \rangle$ also give a contribution here (for simplicity we have dropped the time variable). The contribution of the anomalous expectation values after splitting it into its real and imaginary part is

$$\langle \delta \phi_{\mathbf{q}}^* \delta \phi_{-\mathbf{q}}^* \rangle + \langle \delta \phi_{\mathbf{q}} \delta \phi_{-\mathbf{q}} \rangle = 2 \left(\langle (\delta \phi_{\mathbf{k}}')^2 \rangle - \langle (\delta \phi_{\mathbf{k}}'')^2 \rangle \right),$$

such that the static structure factor is given as

$$\begin{aligned} S(\mathbf{q}) &= 1 + 2 \frac{N_0}{N_{\text{tot}}} \langle n_{\mathbf{q}} \rangle + \frac{N_0}{N_{\text{tot}}} \left(\langle \delta \phi_{\mathbf{q}}^* \delta \phi_{-\mathbf{q}}^* \rangle + \langle \delta \phi_{\mathbf{q}} \delta \phi_{-\mathbf{q}} \rangle \right) + \sum_{\mathbf{k} \neq \{0, -\mathbf{q}\}} \langle n_{\mathbf{k}} \rangle \langle n_{\mathbf{k}+\mathbf{q}} \rangle = \\ &= 1 + 4 \frac{N_0}{N_{\text{tot}}} \langle (\delta \phi_{\mathbf{q}}')^2 \rangle + \sum_{\mathbf{k} \neq \{0, -\mathbf{q}\}} \langle n_{\mathbf{q}} \rangle \langle n_{\mathbf{k}+\mathbf{q}} \rangle. \end{aligned} \quad (126)$$

After performing the limit $M \rightarrow \infty$ we find

$$\langle (\delta \phi_{\mathbf{q}}')^2 \rangle = \lim_{M \rightarrow \infty} \frac{1}{2} [\hat{A}^{(\mathbf{q})}]_{11}^{-1} = -\frac{1}{4} + \frac{1}{4} \frac{\epsilon_{\mathbf{q}}}{E_{\mathbf{q}}} \coth \left(\frac{\beta}{2} E_{\mathbf{q}} \right). \quad (127)$$

If we neglect the last term in Eq. (126) which is quadratic in the momentum distribution, this expression reduces to

$$S(\mathbf{q}) = \frac{\epsilon_{\mathbf{q}}}{E_{\mathbf{q}}} \coth \left(\frac{\beta}{2} E_{\mathbf{q}} \right). \quad (128)$$

$$S(\mathbf{q}) = \epsilon_{\mathbf{q}}/E_{\mathbf{q}}.$$

To determine the type of the decay of the density-density correlations for large distances (i.e. exponentially or algebraically) at zero temperature in d dimensions in the BEC phase, we Fourier transform the static structure factor for small wave vectors, because they are relevant for large distances \mathbf{r} :

$$D(\mathbf{r}) \sim \int S(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}} d^d q \sim \int \frac{\mathbf{q}^2}{\sqrt{2(\mu + J)\mathbf{q}^2 + \mathbf{q}^4}} e^{i\mathbf{q} \cdot \mathbf{r}} d^d q \sim \int \frac{|\mathbf{q}|}{\sqrt{2(\mu + J)}} e^{i\mathbf{q} \cdot \mathbf{r}} d^d q. \quad (129)$$

This expression shows an algebraic decay. In $d = 1$ the decay is proportional to $1/r^2$ (in agreement with the result (96) of the one-dimensional system), in $d = 2$ it decays like $1/r^3$, and in $d = 3$ like $1/r^4$ (see Appendix D). In the empty phase, all CFs vanish completely at zero temperature. Thus, the static structure factor is constantly unity.

5 Strongly interacting bosons in the dense regime

5.1 Paired-fermion model

5.1.1 Bosonic molecules of spin-1/2 fermions

We now introduce a model of hard-core bosons which are constructed by molecules consisting of pairs of spin-1/2 fermions, as an alternative to the hard-core boson model. In order to distinguish it from the latter this model will be referred to as “paired-fermion model”.

A general model which was introduced to study the dissociation of bosonic molecules into pairs of fermionic atoms in an optical lattice was proposed in ref. [58]. It is given by the Hamiltonian

$$\hat{H} - \mu \hat{N}_{\text{tot}} = -\frac{\bar{t}}{2d} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \sum_{\sigma=\uparrow, \downarrow} \hat{c}_{\mathbf{r}, \sigma}^+ \hat{c}_{\mathbf{r}', \sigma} - \frac{J}{2d} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{c}_{\mathbf{r}, \uparrow}^+ \hat{c}_{\mathbf{r}', \uparrow} \hat{c}_{\mathbf{r}, \downarrow}^+ \hat{c}_{\mathbf{r}', \downarrow} - \mu \sum_{\mathbf{r}} \sum_{\sigma=\uparrow, \downarrow} \hat{c}_{\mathbf{r}, \sigma}^+ \hat{c}_{\mathbf{r}, \sigma}. \quad (130)$$

The index $\sigma = \uparrow, \downarrow$ denotes the spin. The first term describes tunneling of individual fermions with rate \bar{t} and the second term tunneling of local fermion pairs. Similar Hamiltonians were proposed in a couple of works for homogeneous systems, in order to study the BEC-BCS crossover [59, 60, 61]. In contrast to the lattice-Hamiltonian (130) they do not exhibit a Mott insulating phase.

Because the main interest here shall be the model of hard-core bosons, we consider the case $\bar{t} = 0$ in the following, i.e. we exclude the existence of dissociated fermionic atoms. Further we will write the index $\sigma = 1, 2$ as superscript instead of the spin indices \uparrow, \downarrow . We write the grand canonical partition function of the system in terms of a fermionic functional integral of a field of conjugate Grassmann variables as defined in Eq. (37) with the action

$$A_{\text{ferm}}(\bar{\psi}, \psi) = \sum_{n=1}^M \left\{ \sum_{\mathbf{r}, \sigma} \bar{\psi}_{\mathbf{r}, n+1}^{\sigma} (\psi_{\mathbf{r}, n+1}^{\sigma} - \psi_{\mathbf{r}, n}^{\sigma}) - \frac{1}{2} \frac{\beta \mu}{M} \sum_{\mathbf{r}, \sigma} \bar{\psi}_{\mathbf{r}, n+1}^{\sigma} \psi_{\mathbf{r}, n}^{\sigma} \right. \\ \left. + \frac{\beta}{M} \sum_{\mathbf{r}, \mathbf{r}'} \hat{J}_{\mathbf{r}\mathbf{r}'} \bar{\psi}_{\mathbf{r}, n+1}^1 \psi_{\mathbf{r}', n}^1 \bar{\psi}_{\mathbf{r}, n+1}^2 \psi_{\mathbf{r}', n}^2 \right\}, \quad (131)$$

with anti-periodic boundary conditions in time. Here, we have replaced $\mu \rightarrow \mu/2$ due to the fact that the chemical potential is associated with the number of *paired* fermions (i.e. to the bosonic molecules), hence the factor 1/2 in front of the term which contains μ , while in Eq. (130), \hat{N}_{tot} is the particle number operator of single fermions.

In the world-line picture, the paired-fermion model given by A_{ferm} is represented by pairs of fermions with opposite spin 1 and 2 whose world-lines always stay together while they tunnel through the lattice. Tunneling of unpaired fermions does not exist. The world-lines of two fermions of species 1 and 2 always stick together while tunneling through the lattice.

5.1.2 Hubbard-Stratonovich decoupling

The idea of a Hubbard-Stratonovich transformation is to decouple a quartic term of a many-body system by writing it in terms of a Gaussian integral [62]. The original field variables are then only of second order and can be integrated out such that the system is represented only by the field variables of the Gaussian integral.

We perform a Hubbard-Stratonovich transformation on the system of paired fermions [58] given by Eq. (131). Only the term which describes hopping of fermion pairs is quartic, so we will decouple it. Contrary to the case of the hard-core boson model, it is not necessary here to decouple the entire off-diagonal term, because the term describing the discrete-time derivative and the term containing the chemical potential are already of second order. For the matrix with fermionic boundary conditions we write

$$\hat{v}_{\mathbf{r}\mathbf{r}';nm}^{\text{ferm}} = (\delta_{n,m+1} - \delta_{n1}\delta_{mM}) \frac{\beta}{M} \hat{J}_{\mathbf{r}\mathbf{r}'} + s \delta_{nm} , \quad (132)$$

and insert the identity

$$\begin{aligned} & \text{const.} \times \exp \left\{ -\frac{\beta}{M} \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m=1}^M \hat{J}_{\mathbf{r}\mathbf{r}'} \bar{\psi}_{\mathbf{r},n+1}^1 \psi_{\mathbf{r}',n}^1 \bar{\psi}_{\mathbf{r},n+1}^2 \psi_{\mathbf{r}',n}^2 \right\} \\ &= \int \exp \left\{ -\frac{\beta}{M} \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \varphi_{\mathbf{r},n}^* (\hat{v}_{\mathbf{r}\mathbf{r}';nm}^{\text{ferm}})^{-1} \varphi_{\mathbf{r}',m} - \frac{1}{s} \sum_{\mathbf{r},n} \chi_{\mathbf{r},n}^* \chi_{\mathbf{r},n} \right. \\ & \quad \left. + \sum_{\mathbf{r},n} [\psi_{\mathbf{r},n}^2 \psi_{\mathbf{r},n}^1 (i\varphi_{\mathbf{r},n}^* + \chi_{\mathbf{r},n}^*) + \bar{\psi}_{\mathbf{r},n+1}^1 \bar{\psi}_{\mathbf{r},n+1}^2 (i\varphi_{\mathbf{r},n} + \chi_{\mathbf{r},n})] \right\} \prod_{\mathbf{r},n} \frac{d\varphi_{\mathbf{r},n}^* d\varphi_{\mathbf{r},n} d\chi_{\mathbf{r},n}^* d\chi_{\mathbf{r},n}}{(2\pi i)^2} . \end{aligned} \quad (133)$$

The parameter s cares for the convergence of the integral of the complex field φ . For $\hat{v}_{\mathbf{r}\mathbf{r}';nm}^{\text{ferm}}$ we have the eigenvalues

$$v_{\mathbf{k},n}^{\text{ferm}} = e^{-i\frac{2\pi}{M}(n-\frac{1}{2})} \frac{\beta}{M} \tilde{\epsilon}_{\mathbf{k}} + s , \quad (134)$$

therefore one has to choose s large enough such that all eigenvalues are non-negative, but besides this condition the choice of s is free. We integrate out the Grassmann field in the functional integral representation of the partition function, like we did in the previous section:

$$Z_{\text{ferm}} = \int \exp [-\tilde{A}_{\text{ferm}}(\varphi^*, \varphi, \chi^*, \chi)] \prod_{\mathbf{r},n} \frac{d\varphi_{\mathbf{r},n}^* d\varphi_{\mathbf{r},n} d\chi_{\mathbf{r},n}^* d\chi_{\mathbf{r},n}}{(2\pi i)^2} \quad (135)$$

with the action

$$\tilde{A}_{\text{ferm}}(\varphi^*, \varphi, \chi^*, \chi) = \sum_{\mathbf{r},\mathbf{r}'} \sum_{n,m} \varphi_{\mathbf{r},n}^* (\hat{v}_{\mathbf{r}\mathbf{r}';nm}^{\text{ferm}})^{-1} \varphi_{\mathbf{r}',m} + \frac{1}{s} \sum_{\mathbf{r},n} \chi_{\mathbf{r},n}^* \chi_{\mathbf{r},n} - \sum_{\mathbf{r}} \log \det \hat{\mathbb{G}}_{\mathbf{r}}^{-1} , \quad (136)$$

where we have introduced the matrix

$$\begin{aligned} \hat{\mathbb{G}}_{\mathbf{r}}^{-1} &= \delta_{nm} \begin{pmatrix} i\varphi_{\mathbf{r},n} + \chi_{\mathbf{r},n} & 1 \\ 1 & -(i\varphi_{\mathbf{r},n}^* + \chi_{\mathbf{r},n}^*) \end{pmatrix} \\ & \quad - (\delta_{n,m+1} - \delta_{n1}\delta_{mM}) \begin{pmatrix} 0 & 1 + \frac{\beta\mu}{2M} \\ 1 - \frac{\beta\mu}{2M} & 0 \end{pmatrix} . \end{aligned} \quad (137)$$

5.1.3 Saddle-point expansion

Under the assumption

$$\varphi_{\mathbf{r},n}^* \equiv \varphi_0^* \quad \varphi_{\mathbf{r},n} \equiv \varphi_0 \quad \chi_{\mathbf{r},n}^* \equiv \chi_0^* \quad \chi_{\mathbf{r},n} \equiv \chi_0 \quad (138)$$

that the mean-field solution is constant in space and time, we can Fourier transform the matrix $\hat{\mathbf{G}}_{\mathbf{r},n}^{-1} \equiv \hat{\mathbf{G}}_n^{-1}$ in Eq. (137) with respect to the discrete-time index:

$$\hat{\mathbf{G}}_n^{-1} = \begin{pmatrix} i\varphi_0 + \chi_0 & 1 - e^{-\frac{i2\pi}{M}(n-\frac{1}{2})} \left(1 + \frac{\beta\mu}{2M}\right) \\ 1 - e^{-\frac{i2\pi}{M}(n-\frac{1}{2})} \left(1 - \frac{\beta\mu}{2M}\right) & -(i\varphi_0^* + \chi_0^*) \end{pmatrix}. \quad (139)$$

By the use of the identity $\sum_{\mathbf{r}',m} (\hat{v}_{\mathbf{r}\mathbf{r}';nm}^{\text{ferm}})^{-1} = (s - \beta J/M)^{-1}$ we have:

$$\begin{aligned} \frac{\tilde{A}_0^{\text{ferm}}}{\mathcal{N}M} &= \frac{\varphi_0^* \varphi_0}{s + \frac{\beta J}{M}} + \frac{1}{s} \chi_0^* \chi_0 \\ &- \frac{1}{M} \sum_{n=1}^M \log \left[-(i\varphi_0 + \chi_0)(i\varphi_0^* + \chi_0^*) - 1 - e^{-2\frac{i2\pi}{M}(n-\frac{1}{2})} \left(1 - \left(\frac{\beta\mu}{2M}\right)^2\right) + 2e^{-\frac{i2\pi}{M}(n-\frac{1}{2})} \right]. \end{aligned} \quad (140)$$

From the saddle point conditions

$$\frac{\partial \tilde{A}_{\text{ferm}}}{\partial \varphi_{\mathbf{r},n}^*} = \frac{\partial \tilde{A}_{\text{ferm}}}{\partial \varphi_{\mathbf{r},n}} = 0, \quad \frac{\partial \tilde{A}_{\text{ferm}}}{\partial \chi_{\mathbf{r},n}^*} = \frac{\partial \tilde{A}_{\text{ferm}}}{\partial \chi_{\mathbf{r},n}} = 0 \quad (141)$$

we find the mean-field equations

$$\frac{\chi_0}{s} = -iG, \quad \frac{\varphi_0}{s + \frac{\beta J}{M}} = G, \quad (142)$$

where G is calculated in Appendix A.5 and the result is

$$G = \frac{J\varphi_0/s}{\sqrt{\mu^2 + \left(\frac{J|\varphi_0|}{s}\right)^2}} \tanh \left[\frac{\beta}{2} \sqrt{\mu^2 + \left(\frac{J|\varphi_0|}{s}\right)^2} \right]. \quad (143)$$

We find a trivial solution with $\varphi_0 = \varphi_0^* = \chi_0 = \chi_0^* = 0$ and a non-trivial solution with broken $U(1)$ symmetry. For the mean-field action we find (after integrating G with respect to $i\varphi_0 + \chi_0$):

$$\tilde{A}_0^{\text{ferm}} = \mathcal{N} \left[\frac{\beta J}{s^2} |\varphi_0|^2 - \frac{\beta\mu}{2} - \log \cosh \left(\frac{\beta}{2} \sqrt{\mu^2 + \left(\frac{J|\varphi_0|}{s}\right)^2} \right) \right]. \quad (144)$$

The complex fields φ and χ are expected to fluctuate about the SP solution due to thermal and quantum effects. If we keep our expressions only to the first order of $\tau = \beta/M$, making use of the notation $\partial_\tau = (\delta_{n,m+1} - \delta_{n,m})/\tau$ and denoting $\Delta = i\phi + \chi$ and $\bar{\Delta} = i\phi^* + \chi^*$, then

$$\hat{\mathbf{G}}^{-1} = \hat{\mathbf{G}}_0^{-1} + \begin{pmatrix} \delta\Delta & 0 \\ 0 & -\delta\bar{\Delta} \end{pmatrix}, \quad (145)$$

where

$$\hat{\mathbf{G}}_0^{-1} = \begin{pmatrix} \Delta_0 & \tau(\partial_\tau - \mu) \\ \tau(\partial_\tau + \mu) & -\bar{\Delta}_0 \end{pmatrix}.$$

Applying the Taylor expansion $\ln(1+x) = x - x^2/2 + \dots$ we get

$$\begin{aligned} \log \det \hat{\mathbf{G}}^{-1} &= \text{tr} \ln \hat{\mathbf{G}}^{-1} = \text{tr} \ln \left[\hat{\mathbf{G}}_0^{-1} + \begin{pmatrix} \delta\Delta & 0 \\ 0 & -\delta\bar{\Delta} \end{pmatrix} \right] \approx \\ &\approx \text{tr} \ln \hat{\mathbf{G}}_0^{-1} - \frac{1}{2} \text{tr} \left[\hat{\mathbf{G}}_0 \begin{pmatrix} \delta\Delta & 0 \\ 0 & -\delta\bar{\Delta} \end{pmatrix} \right]^2. \end{aligned} \quad (146)$$

Calculating the trace in $p = \{q, \omega\}$ representation we get

$$Z \sim \int D[\delta\varphi] \exp \left[-\delta\tilde{A}^{\text{ferm}} \right], \quad (147)$$

where $\delta\tilde{A}^{\text{ferm}}$ is given by

$$\delta\tilde{A}^{\text{ferm}} = \sum_{\mathbf{k}} \sum_{n,m} \delta\varphi_{\mathbf{k},n}^* \left(\hat{\mathcal{G}}_{\mathbf{k};nm} \right)^{-1} \delta\varphi_{\mathbf{k},m}. \quad (148)$$

Here, $\hat{\mathcal{G}}$ represents the Green's function of quasiparticle fluctuations (Appendix E).

5.1.4 Results for the paired-fermion model

It turns out that even on the mean-field level, the paired-fermion model shows some interesting physical results. The condensate density we get via the definition (52) and the mean-field approximation that the CF factorizes for large distances:

$$n_0 = \lim_{\mathbf{r}-\mathbf{r}' \rightarrow \infty} \langle \bar{\psi}_{\mathbf{r},n+1}^1 \bar{\psi}_{\mathbf{r},n+1}^2 \psi_{\mathbf{r}',n}^2 \psi_{\mathbf{r}',n}^1 \rangle = \langle \bar{\psi}_{\mathbf{r},n+1}^1 \bar{\psi}_{\mathbf{r},n+1}^2 \rangle \langle \psi_{\mathbf{r}',n}^2 \psi_{\mathbf{r}',n}^1 \rangle. \quad (149)$$

Further, the CFs which are of second order in the Grassmann field, are given by the diagonal elements of the matrix $\hat{\mathbf{G}}$ whose inverse is given in Eq. (137). These diagonal elements are equal to $G/2$ from Eq. (143):

$$\langle \bar{\psi}_{\mathbf{r},n+1}^1 \bar{\psi}_{\mathbf{r},n+1}^2 \rangle = \langle \psi_{\mathbf{r}',n}^2 \psi_{\mathbf{r}',n}^1 \rangle = \frac{G}{2} \implies n_0 \equiv \frac{G^2}{4}. \quad (150)$$

Thus, from the Eqs. (143) and (150), together with the $M \rightarrow \infty$ limit of Eq. (142), one finds a self-consistent equation for the condensate density:

$$J = \sqrt{\mu^2 + 4J^2 n_0} \coth \left[\frac{\beta}{2} \sqrt{\mu^2 + 4J^2 n_0} \right]. \quad (151)$$

The total particle density we get from the mean-field action (144) is

$$n_{\text{tot}} = -\frac{1}{\beta\mathcal{N}} \frac{\partial \tilde{A}_0^{\text{ferm}}}{\partial \mu} = \frac{1}{2} + \frac{1}{2} \frac{\mu}{\sqrt{\mu^2 + 4J^2 n_0}} \tanh \left[\frac{\beta}{2} \sqrt{\mu^2 + 4J^2 n_0} \right] \quad (152)$$

$$= \begin{cases} \frac{1}{2} \left(1 + \frac{\mu}{J} \right) & \text{in the condensed phase } (n_0 > 0) \\ \frac{1}{2} \left[1 + \tanh \left(\frac{\beta\mu}{2} \right) \right] & \text{in the non-condensed phase } (n_0 = 0). \end{cases} \quad (153)$$

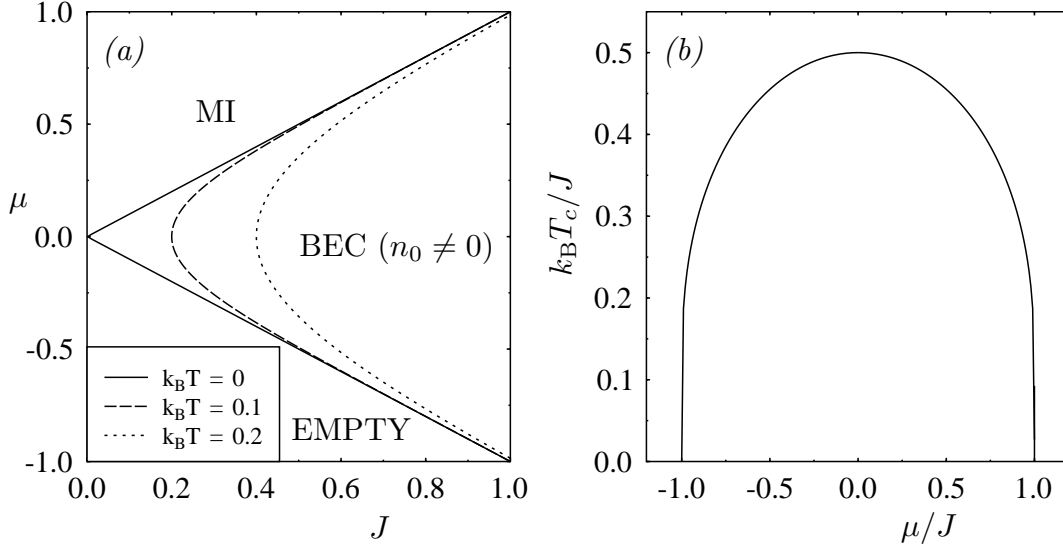


Fig. 9 (a) Phase diagram with phase boundaries between the BEC and the non-condensed phase for different temperatures. For $k_B T \neq 0$ there is only one phase boundary between a BEC and a non-condensed phase. The energy unit is arbitrary because of a simple scaling behaviour. (b) Critical temperature of BEC formation.

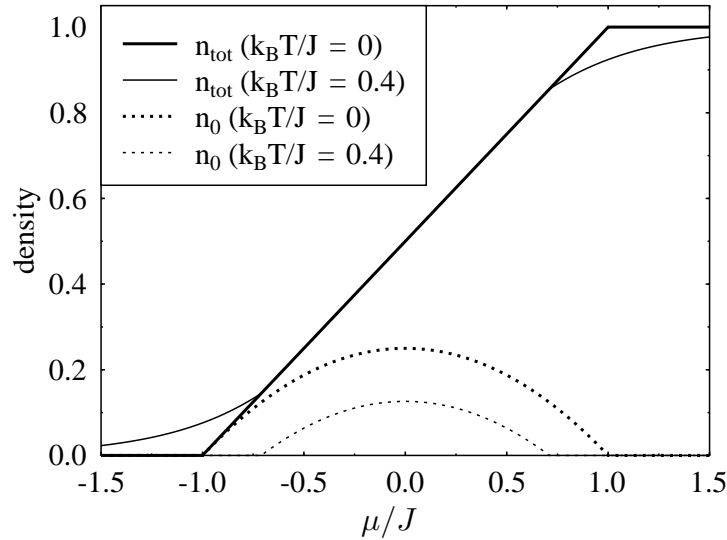


Fig. 10 Total particle density and condensate density for zero temperature (thick lines, given by Eqs. (154) and (155)) and for non-zero temperature (thin lines) plotted against chemical potential.

It might be interesting to mention that all these mean-field results do not depend on the parameter s which was introduced in the Hubbard-Stratonovich transformation for the convergence of the Gaussian integral.

The phase boundary between the BEC and the non-condensed phase we get from Eq. (151). The resulting phase diagram is depicted in Fig. 9. We see in picture (a) that for $T > 0$ the phase diagram is separated into two parts, a BEC phase and a non-condensed phase. But at $T = 0$ there are three phases: A

BEC, an empty phase ($n_{\text{tot}} = 0$) for $\mu < -J$, and a Mott-insulator ($n_{\text{tot}} = 1$) for $\mu > J$. A density profile of n_{tot} and n_0 is plotted in Fig. 10 for different temperatures. At zero temperature the sharp transitions between the empty phase and the BEC, and the BEC and the MI, can be seen in the plot of the total particle density. The zero temperature result is

$$n_0 = \begin{cases} \frac{1}{4} \left(1 - \frac{\mu^2}{J^2}\right) & \text{if } -J < \mu < J \\ 0 & \text{else} \end{cases}, \quad (154)$$

$$n_{\text{tot}} = \begin{cases} 0 & \text{if } \mu \leq -J \\ \frac{1}{2} \left(1 - \frac{\mu}{J}\right) & \text{if } -J < \mu < J \\ 1 & \text{if } J \leq \mu \end{cases}. \quad (155)$$

If the temperature increases, the sharp transitions are smeared out.

Calculations for the quasiparticle spectrum by finding the poles of the Green's matrix $\hat{\mathcal{G}}$ of the Gaussian fluctuations have been made for the zero temperature phase diagram [63]. The zero temperature result in the empty phase and in the MI phase is

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + |\mu| - J, \quad (156)$$

with the gap $\Delta = |\mu| - J$, and in the BEC phase it is

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} \left[J \left(1 - \left(\frac{\mu}{J}\right)^2\right) + \left(\frac{\mu}{J}\right)^2 \epsilon_{\mathbf{k}} \right]}. \quad (157)$$

In the dilute regime, i.e. if $\mu = -J + \Delta\mu$, with $\Delta\mu \ll J$, this can be approximated by

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}(2(\mu + J) + \epsilon_{\mathbf{k}})}. \quad (158)$$

Using the Green's function of quasiparticle fluctuations (see Appendix E), we can calculate the effect of quantum fluctuations on the condensate density:

$$n_0 = \frac{1}{4} \left(1 - \frac{\mu^2}{J^2}\right) + \delta n_0, \quad (159)$$

where the correction to the mean-field result is

$$\begin{aligned} \delta n_0 = & -\frac{(J^2 - \mu^2)\mu^2}{J^3} \int \frac{d^d k}{(2\pi)^d} \frac{B_{\mathbf{k}}^2 g_{\mathbf{k}}}{E_{\mathbf{k}}} + \frac{(J^2 - \mu^2)}{4J^3} \int \frac{d^d k}{(2\pi)^d} B_{\mathbf{k}} E_{\mathbf{k}} - \frac{(J^2 - \mu^2)^2}{4J^3} \int \frac{d^d k}{(2\pi)^d} \frac{B_{\mathbf{k}}^2}{E_{\mathbf{k}}} + \\ & + \frac{3(J^2 - \mu^2)^2 \mu^2}{4J^5} \int \frac{d^d k}{(2\pi)^d} \frac{B_{\mathbf{k}}^2 g_{\mathbf{k}}}{E_{\mathbf{k}}}, \end{aligned} \quad (160)$$

where $B_{\mathbf{k}} = \frac{1}{d} \sum_{j=1}^d \cos k_j$, $g_{\mathbf{k}} = 1 - B_{\mathbf{k}}$. It should be noticed that this correction vanishes at the critical point.

It might be interesting to mention that in the zero temperature limit near the phase transition to the empty phase where $\mu = -J + \Delta\mu$ with $\Delta\mu \ll J$, i.e. in the dilute regime, it is possible to approximate

$$n_0 = \frac{\Delta\mu}{2J} + \mathcal{O}(\Delta\mu^2) = n_{\text{tot}} + \mathcal{O}(\Delta\mu^2). \quad (161)$$

This agrees with the Gross-Pitaevskii result (103), if the term of order $\Delta\mu^2$ is neglected, and the identification $g \equiv 2J$ has been made.

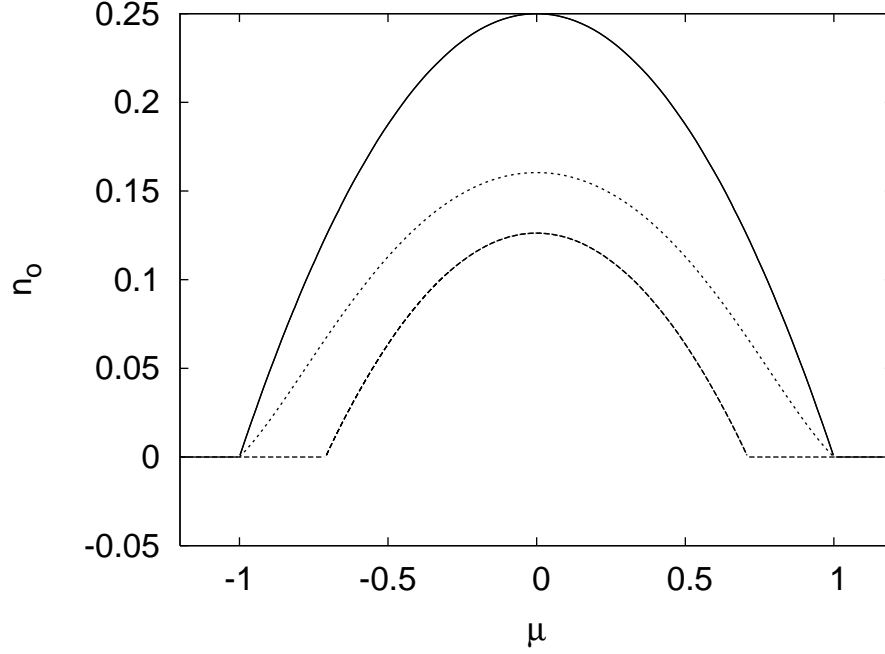


Fig. 11 Condensate density. The solid, dotted and dashed lines show the mean-field result at $T = 0$, the influence of quantum fluctuations at $T = 0$ to the mean-field result and the mean-field result at $T = 0.2$, respectively.

The main correction due to the thermal fluctuations are already included in our mean-field theory, where the condensed density is given by

$$n_0 = \frac{|\varphi_0|^2}{4J^2}, \quad (162)$$

and $|\varphi_0|^2$ can be determined from Eqs. (142-143).

The effect of quantum fluctuations and thermal fluctuations is depicted in Fig. 11. We see that both of them lead to a depletion of the condensate, but the quantum depletion alone does not change the transition points.

The static structure factor for small wave vector \mathbf{q} and for small temperature T in the BEC phase reads

$$S(\mathbf{q}) \sim \frac{(J^2 - \mu^2)}{J^2 n} \frac{Jg_{\mathbf{q}}}{E_{\mathbf{q}}} \coth \frac{\beta E_{\mathbf{q}}}{2}, \quad (163)$$

where n is a total density of particles.

In the dilute regime, i.e. close to the empty phase, when $n \sim (J + \mu)/J$ and $J - \mu \approx 2J$ we obtain

$$S(\mathbf{q}) \sim \frac{Jg_{\mathbf{q}}}{E_{\mathbf{q}}} \coth \frac{\beta E_{\mathbf{q}}}{2}, \quad (164)$$

which is in agreement with the well-known result for the weakly interacting Bose gas (cf. section 4. In the dense regime, i.e. close to the Mott phase when $n \approx 1$, the static structure factor vanishes.

In conclusion, we can say that the paired-fermion model has three phases at zero temperature, an empty phase, a MI, and a BEC, even on the mean-field level. However, at non-zero temperatures a new phase emerges from the MI phase and the empty phase, that is controlled by thermal fluctuations.

5.2 Slave-boson model

5.2.1 Hamiltonian and functional integral

In this chapter it shall be shown that a slave-boson approach can be applied to describe a system of hard-core bosons. The slave-boson representation was originally developed for fermion systems, e.g. the Hubbard model [64, 65]. It allows to account for many aspects of strong correlations even on the mean-field level. The slave-boson approach to hard-core bosons that will be presented here, has been developed in refs. [66, 67, 68, 69]. It is an alternative to the paired-fermion model which was discussed in the previous chapter.

Again, the starting point is the Hamiltonian (27). We introduce bosonic creation and annihilation operators of empty (\hat{e}_r^+ , \hat{e}_r) and occupied (\hat{b}_r^+ , \hat{b}_r) sites which act on a fictitious “vacuum”. To transfer the Hamiltonian to the extended Fock space, we replace the hard-core boson operators by

$$\hat{a}_r^+ \rightarrow \hat{b}_r^+ \hat{e}_r \quad ; \quad \hat{a}_r \rightarrow \hat{e}_r^+ \hat{b}_r . \quad (165)$$

Then the Hamiltonian (27) is replaced by the slave-boson Hamiltonian as

$$\hat{H}_{\text{hc}} \rightarrow \hat{H}_{\text{sb}} = -\frac{J}{2d} \sum_{\langle r, r' \rangle} \hat{b}_r^+ \hat{e}_r \hat{e}_{r'}^+ \hat{b}_{r'} + \sum_r V_r \hat{b}_r^+ \hat{b}_r . \quad (166)$$

A hopping process can be understood as a swapping of an occupied site and an empty site. The occupation number operator of site r is $\hat{b}_r^+ \hat{b}_r$. It should be noticed that the external potential acts only on the particles but not on the empty sites. To assure that a lattice site r is either empty or occupied by a boson, we impose the constraint

$$\hat{b}_r^+ \hat{b}_r + \hat{e}_r^+ \hat{e}_r = 1 . \quad (167)$$

A similar theory for the Bose-Hubbard model has been established in refs. [70, 71]. In this case, an infinite number of operators $(\hat{b}_r^\alpha)^+$, \hat{b}_r^α for each occupation number α has to be introduced at each lattice site, because multiple occupation is possible. In this respect, the slave-boson approach for hard-core bosons is much simpler. However, the hard-core boson model describes a projection of the full Bose-Hubbard model to n and $n+1$ bosons per site, as discussed in the Introduction 1.4.

The grand canonical partition function of the system can be expressed as a functional integral with two complex fields $b_r(\tau)$ and $e_r(\tau)$. For the following mean-field calculation, we use the classical approximation here, which only takes into account thermal fluctuations but not quantum fluctuations. This means that for the fields in Matsubara representation

$$b_r(\tau) = \frac{1}{\sqrt{\beta}} \sum_n b_{r,n} e^{i\omega_n \tau} ; \quad e_r(\tau) = \frac{1}{\sqrt{\beta}} \sum_n e_{r,n} e^{i\omega_n \tau} ,$$

with bosonic Matsubara frequencies ω_n , only the terms with $\omega_0 = 0$ are taken into account, if one assumes that

$$e_{r,\omega_n} \approx e_{r,\omega_n} \approx 0 , \quad \text{if } n \neq 0 . \quad (168)$$

In other words, the time dependence of the fields is neglected. This is justified if we can assume that quantum fluctuations (which are neglected in the classical approximation) are small.

The constraint $|b_r|^2 + |e_r|^2 = 1$ is enforced by a δ -function in the integration measure:

$$Z_{\text{sb}} = \int e^{-A[b, b^*, e, e^*]} \mathcal{D}[b, b^*, e, e^*] , \quad (169)$$

with

$$\mathcal{D}[b, b^*, e, e^*] = \prod_{\mathbf{r}} (|b_{\mathbf{r}}|^2 + |e_{\mathbf{r}}|^2 - 1) db_{\mathbf{r}} db_{\mathbf{r}}^* de_{\mathbf{r}} de_{\mathbf{r}}^* \quad (170)$$

and the action

$$A[b, b^*, e, e^*] = \beta \left\{ - \sum_{\mathbf{r}} \mu_{\mathbf{r}} b_{\mathbf{r}}^* b_{\mathbf{r}} - \frac{J}{2d} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} b_{\mathbf{r}}^* e_{\mathbf{r}} e_{\mathbf{r}'}^* b_{\mathbf{r}'} \right\}. \quad (171)$$

Here, we consider a space-dependent chemical potential $\mu_{\mathbf{r}} = \mu - V_{\mathbf{r}}$.

5.2.2 Two-fluid theory in classical approximation

The hopping term of the action is of fourth order in the field variables. Therefore it is not possible to perform the integration directly. However, it is possible to decouple the hopping term by introducing two new fields, a complex field Φ and a real field φ , and perform a Hubbard-Stratonovich transformation. The fields b and e can be integrated out then, and a mean-field approximation can be applied to the fields Φ and φ [69].

The idea of the Hubbard-Stratonovich decoupling is similar to the one used in the previous chapter to decouple the fourth order terms of the Grassmann fields. We insert the identity

$$\begin{aligned} \text{const.} \times e^{-A[b, b^*, e, e^*]} &= \int \exp \left\{ -\beta \left[\sum_{\mathbf{r}, \mathbf{r}'} \Phi_{\mathbf{r}}^* \left[\frac{s - \hat{J}}{s^2} \right]_{\mathbf{r}\mathbf{r}'}^{-1} \Phi_{\mathbf{r}} + s \sum_{\mathbf{r}} \varphi_{\mathbf{r}}^2 \right. \right. \\ &\quad \left. \left. + \sum_{\mathbf{r}} (e_{\mathbf{r}}, b_{\mathbf{r}}) \begin{pmatrix} 2s\varphi_{\mathbf{r}} + s & s\Phi_{\mathbf{r}} \\ s\Phi_{\mathbf{r}}^* & -\mu_{\mathbf{r}} \end{pmatrix} \begin{pmatrix} e_{\mathbf{r}}^* \\ b_{\mathbf{r}}^* \end{pmatrix} \right] \right\} \mathcal{D}[\Phi^*, \Phi, \varphi], \end{aligned} \quad (172)$$

with the integration measure

$$\mathcal{D}[\Phi^*, \Phi, \varphi] = \prod_{\mathbf{r}} \frac{d\Phi_{\mathbf{r}}^* d\Phi_{\mathbf{r}} d\varphi_{\mathbf{r}}}{(2\pi)^{3/2}}. \quad (173)$$

Here, \hat{J} is the hopping matrix (76). The constant factor is of no physical relevance. Like for the paired-fermion model which was discussed before, the parameter s takes care of the convergence of the Gaussian integral. It has the unit of an energy and should not be too small compared to J . Although the exact identity does not depend on s , we will see subsequently that the mean-field equation we will derive, does. This is a difference to the previously discussed model, where the result which was derived on the mean-field level and on the level of Gaussian fluctuations, did not depend on the free parameter s .

After substituting the identity (172) into the functional integral (171), the fields b and e are only of second order and can be integrated out exactly together with the constraint. This is shown in Appendix F.1. The result for the partition function is

$$Z_{\text{sb}} = \int e^{-\tilde{A}(\Phi^*, \Phi)} \prod_{\mathbf{r}} d\Phi_{\mathbf{r}} d\Phi_{\mathbf{r}}^* \quad (174)$$

with the new action

$$\tilde{A}(\Phi^*, \Phi) = \beta \sum_{\mathbf{r}, \mathbf{r}'} \Phi_{\mathbf{r}}^* \left[\frac{s - \hat{J}}{s^2} \right]_{\mathbf{r}\mathbf{r}'}^{-1} \Phi_{\mathbf{r}'} - \sum_{\mathbf{r}} \log \left[Z'_{\mathbf{r}} e^{\frac{\beta \mu_{\mathbf{r}}}{4}} \right], \quad (175)$$

and the function

$$Z'_{\mathbf{r}} = \int_{-\infty}^{\infty} d\varphi_{\mathbf{r}} \frac{\sinh \left[\beta \sqrt{(\varphi_{\mathbf{r}} s + \frac{\mu_{\mathbf{r}}}{2})^2 + s^2 |\Phi_{\mathbf{r}}|^2} \right]}{\beta \sqrt{(\varphi_{\mathbf{r}} s + \frac{\mu_{\mathbf{r}}}{2})^2 + s^2 |\Phi_{\mathbf{r}}|^2}} e^{-\beta s \varphi_{\mathbf{r}}^2} . \quad (176)$$

Note that the action $\tilde{A}(\Phi^*, \Phi)$ does not depend on the real field φ explicitly, because it appears inside the function Z' only as an integration variable.

The form (174) of the grand canonical partition function can be understood as a two-fluid theory. It is shown in Appendices F.2 and F.3 that the condensate density is related to the field Φ and is given by the relation

$$n_0 \approx \frac{s^2}{(s+J)^2} \lim_{\mathbf{r}-\mathbf{r}' \rightarrow \infty} \langle \Phi_{\mathbf{r}} \Phi_{\mathbf{r}'}^* \rangle , \quad (177)$$

and that the total particle density at site \mathbf{r} is related to the field φ by means of the expectation value

$$n_{\mathbf{r}} = \langle \varphi_{\mathbf{r}} \rangle + \frac{1}{2} . \quad (178)$$

5.2.3 Mean-field theory

A mean-field solution is found by minimising the action via the variational principle $\delta \tilde{A} = 0$, which leads to a saddle-point approximation, as it was done for the paired-fermion model. Since the field φ can be integrated out (e.g. numerically) inside the function $Z'_{\mathbf{r}}$ given in Eq. (176), minimization has to be done with respect to the complex field Φ only:

$$\frac{\partial \tilde{A}}{\partial \Phi_{\mathbf{r}}} = \frac{\partial \tilde{A}}{\partial \Phi_{\mathbf{r}}^*} = 0 . \quad (179)$$

This yields the mean-field equation

$$\sum_{\mathbf{r}'} \left[\frac{s - \hat{J}}{s^2} \right]_{\mathbf{r}\mathbf{r}'}^{-1} \Phi_{\mathbf{r}'} - \frac{1}{\beta} \left[\frac{\partial}{\partial (|\Phi_{\mathbf{r}}|^2)} \log Z'_{\mathbf{r}} \right] \Phi_{\mathbf{r}} = 0 . \quad (180)$$

In the case of a spatially constant field without external trapping potential, i.e. if we assume that $\Phi_{\mathbf{r}} \equiv \Phi_0$ and $\mu_{\mathbf{r}} \equiv \mu$, the mean-field equation is

$$\frac{s^2}{s+J} - \frac{1}{\beta} \frac{\partial}{\partial (|\Phi_0|^2)} \log Z' = 0 . \quad (181)$$

If the field Φ is varying only very slowly between neighbouring lattice sites, we can approximate

$$\sum_{\mathbf{r}'} \left[\frac{s - \hat{J}}{s^2} \right]_{\mathbf{r}\mathbf{r}'}^{-1} \Phi_{\mathbf{r}'} \approx \frac{s^2}{s+J} \Phi_{\mathbf{r}} + \frac{s^2}{(s+J)^2} \sum_{\mathbf{r}'} \left(J \delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'} \right) \Phi_{\mathbf{r}'} . \quad (182)$$

In Fig. 12 the phase boundary between the BEC and the non-condensed phase is plotted for different values of s . The phase boundary solves Eq. (181) for $\Phi_0 = 0$, and has been calculated numerically.

One can see that the BEC phase forms a “bubble” in the phase diagram, if $s/J > 1$. This behaviour is unexpected because the BEC phase should become narrower, if temperature is increased. This means that for too large values of s/J the mean-field theory seems to be incorrect. However, it turns out that the absolute minimum of the action with respect to s at constant J , μ and β occurs at values of $s/J < 1$.

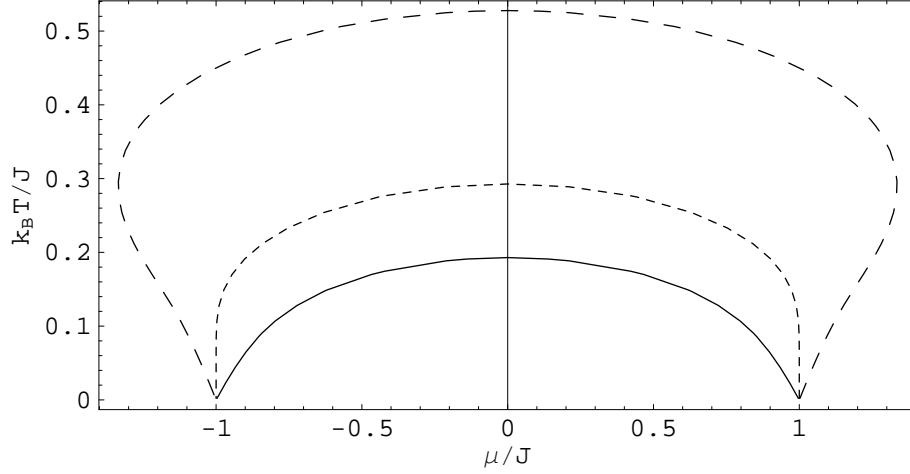


Fig. 12 Phase boundary between the BEC and the non-condensed phase for $s/J = 3$ (long dashes), $s/J = 1$ (short dashes), $s/J = 0.2$ (solid line). Compare these graphs with the graph on the right hand side of Fig. 9, where the critical temperature of the mean-field result for the paired-fermion model is plotted.

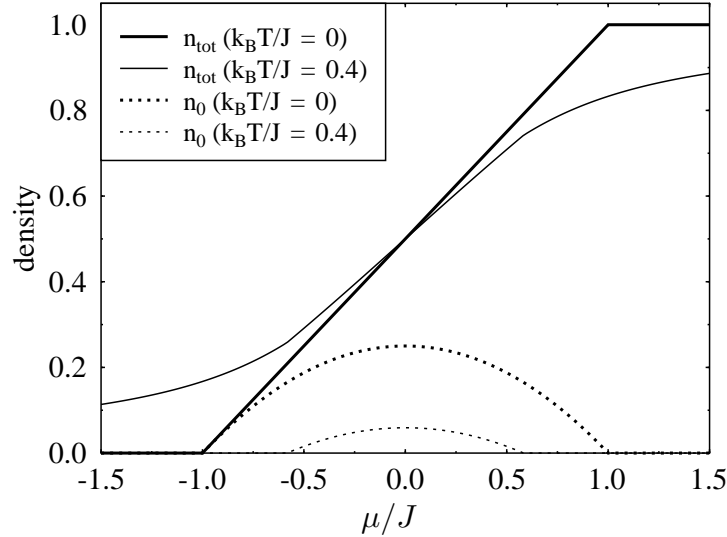


Fig. 13 Total particle density and condensate density for zero temperature (thick lines) and for non-zero temperature (thin lines, $s/J = 1/5.5$) against chemical potential [63]. Compare this graph with the result for the paired-fermion model plotted in Fig. 10.

It is possible to find an exact solution for zero temperature, which does *not* depend on s . This calculation is shown in Appendix F.4. Two phase boundaries are found: A boundary between the BEC and an empty phase with $\mu_c = -J$ and a phase boundary between the BEC and the Mott insulator with $\mu_c = J$. It is identical to the zero temperature mean-field result in Eqs. (154) and (155) that was found for the paired-fermion model, and agrees with it qualitatively at finite temperatures (see Fig. 13). When temperature increases, results strongly depend on s .

5.2.4 Quasiparticle spectrum

We get the quasiparticle spectrum from the Gaussian fluctuations, the same way as it was done for the paired-fermion model. We write

$$\Phi_{\mathbf{r}} = \Phi_0 + \delta\Phi_{\mathbf{r}}, \quad \Phi_{\mathbf{r}}^* = \Phi_0^* + \delta\Phi_{\mathbf{r}}^*,$$

and assume that the fluctuations $\delta\Phi$, $\delta\Phi^*$ about the mean-field solution Φ_0 are small. Substituting this expression into the action (175), and expanding it up to second order in the fluctuations, one finds

$$\tilde{A} = \beta \frac{s^2}{s+J} |\Phi_0|^2 - \log Z'(|\Phi_0|^2) - \frac{\beta}{2} \sum_{\mathbf{r}, \mathbf{r}'} (\delta\Phi_{\mathbf{r}}, \delta\Phi_{\mathbf{r}}^*) \hat{\mathcal{G}}_{\mathbf{r}\mathbf{r}'}^{-1} \begin{pmatrix} \delta\Phi_{\mathbf{r}'}^* \\ \delta\Phi_{\mathbf{r}'} \end{pmatrix}, \quad (183)$$

with the matrix

$$\hat{\mathcal{G}}_{\mathbf{r}\mathbf{r}'}^{-1} = \begin{pmatrix} \frac{J\delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'}}{s+J} + (\tilde{a}_2 + |\Phi_0|^2 \tilde{a}_4) \delta_{\mathbf{r}\mathbf{r}'} & (\Phi_0^*)^2 \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} \\ \Phi_0^2 \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} & \frac{J\delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'}}{s+J} + (\tilde{a}_2 + |\Phi_0|^2 \tilde{a}_4) \delta_{\mathbf{r}\mathbf{r}'} \end{pmatrix}. \quad (184)$$

Here, we have introduced the abbreviations

$$\tilde{a}_2 := -\frac{1}{\beta} \frac{\partial}{\partial(|\Phi|^2)} \log Z' \Big|_{\Phi=\Phi_0} + \frac{s^2}{s+J}, \quad (185)$$

$$\tilde{a}_4 := -\frac{1}{\beta} \frac{\partial^2}{\partial(|\Phi|^2)^2} \log Z' \Big|_{\Phi=\Phi_0}, \quad (186)$$

and used the approximation in Eq. (182). The matrix $\hat{\mathcal{G}}$ has no time-structure because of the classical approximation. To find the Green's function of quasiparticles, we *artificially* introduce the imaginary time by writing

$$\hat{\mathcal{G}}_{\mathbf{r}\mathbf{r}'}^{-1} = \begin{pmatrix} \frac{J\delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'} + \hbar \frac{\partial}{\partial \tau}}{s+J} + \tilde{a}_2 + |\Phi_0|^2 \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} & (\Phi_0^*)^2 \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} \\ \Phi_0^2 \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} & \frac{J\delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'} - \hbar \frac{\partial}{\partial \tau}}{s+J} + \tilde{a}_2 + |\Phi_0|^2 \tilde{a}_4 \delta_{\mathbf{r}\mathbf{r}'} \end{pmatrix}, \quad (187)$$

in analogy with the Bogoliubov theory. After a Fourier transformation it leads to the Green's function

$$\hat{\mathcal{G}}^{-1}(\mathbf{k}, \omega_n) = \frac{s^2}{(s+J)^2} \begin{pmatrix} \epsilon_{\mathbf{k}} + \frac{(s+J)^2}{s^2} \tilde{a}_2 & i\hbar\omega_n \\ i\hbar\omega_n & \epsilon_{\mathbf{k}} + \frac{(s+J)^2}{s^2} (\tilde{a}_2 + 2\tilde{a}_4 |\Phi_0|^2) \end{pmatrix}, \quad (188)$$

which is equivalent to the matrix (114), and $\epsilon_{\mathbf{k}}$ is the lattice dispersion (58). The quasiparticle spectrum is given by the poles of $\hat{\mathcal{G}}$, and can be found by performing the analytic continuation $i\hbar\omega_n \rightarrow E_{\mathbf{k}}$ and solving the equation $\det \hat{\mathcal{G}}^{-1} = 0$. We find solutions for both the BEC phase and the non-condensed phase:

In the BEC phase, where $|\Phi_0|^2 > 0$, the coefficient \tilde{a}_2 vanishes, because Φ_0 solves the mean-field equation (181), which is equivalent to $\tilde{a}_2 = 0$. The solution is

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} \left(2 \frac{(s+J)^2}{s^2} \tilde{a}_4 |\Phi_0|^2 + \epsilon_{\mathbf{k}} \right)}. \quad (189)$$

It is gapless and agrees with the Bogoliubov spectrum (116), when we identify the condensate density with $n_0 = s^2 |\Phi_0|^2 / (s+J)^2$, and the interaction constant with $g = (s+J)^4 \tilde{a}_4 / s^4$. The coefficient \tilde{a}_4 depends on both temperature and chemical potential. Its zero-temperature result is given in Eq. (247) of Appendix F.4. In the dilute gas (i.e. near the phase transition to the empty phase) where $n_0 \ll 1$, we find at zero temperature for the interaction constant the result $g \approx 2J$.

In the non-condensed phase, where $|\Phi_0|^2 = 0$ and $\tilde{a}_2 \neq 0$, the quasiparticle spectrum is gapped, in agreement with the findings of the paired-fermion model:

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Delta, \quad (190)$$

with the gap $\Delta = (s + J)^2 \tilde{a}_2 / s^2$. At zero temperature and near the phase transitions, we find the result $\Delta = |\mu - \mu_c| + \mathcal{O}((\mu - \mu_c)^2)$ which is identical to the zero-temperature result (156) for the paired-fermion model.

5.2.5 Renormalized Gross-Pitaevskii equation

In this section we will derive a mean-field equation which is appropriate to describe the BEC as well as the Mott insulator in a strongly interacting Bose gas, and which is similar to the stationary Gross-Pitaevskii equation. The mean-field equation for a hard-core Bose gas in an optical lattice within the slave-boson approach is given by

$$\frac{s^2}{(s + J)^2} \sum_{\mathbf{r}'} \left(J \delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'} \right) \Phi_{\mathbf{r}'} + \frac{s^2}{s + J} \Phi_{\mathbf{r}} - \frac{1}{\beta} \left[\frac{\partial}{\partial(|\Phi_{\mathbf{r}}|^2)} \log Z'_{\mathbf{r}} \right] \Phi_{\mathbf{r}} = 0. \quad (191)$$

This we get by applying the approximation (182) in Eq. (180). However, it is also possible to describe a system of strongly interacting bosons without lattice potential within this approximation. Therefore we perform a continuum approximation of the hopping term: If the lattice constant a is so small that the order parameter $\Phi_{\mathbf{r}}$ varies only slowly over neighbouring lattice sites, we can treat the 3-dimensional lattice approximately as a continuum:

$$\sum_{\mathbf{r}'} \left(J \delta_{\mathbf{r}\mathbf{r}'} + \hat{J}_{\mathbf{r}\mathbf{r}'} \right) \Phi_{\mathbf{r}'} = -\frac{Ja^2}{6} \sum_{j=1}^3 \frac{\Phi_{\mathbf{r}+a\mathbf{e}_j} - 2\Phi_{\mathbf{r}} + \Phi_{\mathbf{r}-a\mathbf{e}_j}}{a^2} \approx -\frac{Ja^2}{6} \nabla^2 \Phi_{\mathbf{r}}. \quad (192)$$

When working on the continuum, we rescale the order parameter by

$$\Phi(\mathbf{r}) := a^{-3/2} \Phi_{\mathbf{r}}, \quad (193)$$

such that the action (175) can be written as

$$\begin{aligned} \tilde{A}(\Phi^*, \Phi) &= \frac{\beta s^2}{(s + J)^2} \int \left\{ -\frac{Ja^2}{6} \Phi^*(\mathbf{r}) \nabla^2 \Phi(\mathbf{r}) + (s + J) |\Phi(\mathbf{r})|^2 \right. \\ &\quad \left. - \frac{(s + J)^2}{\beta s^2} \log \left[Z'(\mathbf{r}) e^{\frac{\beta \mu(\mathbf{r})}{4}} \right] \right\} d^3 r. \end{aligned} \quad (194)$$

The order parameter is normalized to the number of condensed particles by

$$N_0 = \frac{s^2}{(s + J)^2} \int |\Phi(\mathbf{r})|^2 d^3 r. \quad (195)$$

The replacement (193) has also to be made inside the function Z' , of course. The corresponding mean-field equation for the continuum is

$$\left[-\frac{Ja^2}{6} \nabla^2 + (s + J) - \frac{(s + J)^2}{\beta s^2} \frac{\partial}{\partial(a^3 |\Phi(\mathbf{r})|^2)} \log Z'(\mathbf{r}) \right] \Phi(\mathbf{r}) = 0. \quad (196)$$

The parameters can be identified with those of the conventional GP equation: The mass m of the particles is given by the hopping constant J and the original lattice constant a via

$$\frac{\hbar^2}{2m} \equiv \frac{Ja^2}{6}. \quad (197)$$

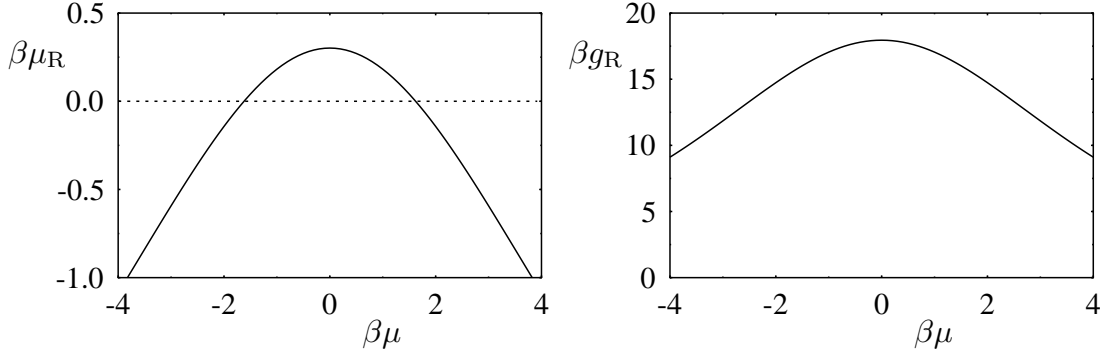


Fig. 14 Coefficients μ_R and g_R of the renormalized GP theory plotted against the chemical potential μ . All parameters are normalised by the inverse temperature β . The tunneling rate was chosen to be $\beta J = 5.5$ and the free parameter was chosen as $s = k_B T$.

In the continuum a loses its identity as lattice constant, but describes a characteristic length scale that can be interpreted as the spacial extension of a boson. Thus, it should be of the same order of magnitude as the s -wave scattering length a_s .

If the order parameter Φ is small, we can expand the potential part of the action up to fourth order:

$$\begin{aligned} & (s + J)a^3|\Phi(\mathbf{r})|^2 - \frac{(s + J)^2}{\beta s^2} \log \left[Z'(\mathbf{r}) e^{\frac{\beta \mu(\mathbf{r})}{4}} \right] \\ &= a_0 - \mu_R |\Phi(\mathbf{r})|^2 + \frac{g_R}{2} \frac{s^2}{(s + J)^2} |\Phi(\mathbf{r})|^4 + \mathcal{O}(|\Phi|^6), \end{aligned} \quad (198)$$

where we have introduced the coefficients

$$a_0 = -\frac{(s + J)^2}{\beta s^2} \log Z'(\mathbf{r})|_{\Phi=0} \quad (199)$$

$$\mu_R = -(s + J) + \frac{(s + J)^2}{\beta s^2} \frac{\partial}{\partial (a^3|\Phi(\mathbf{r})|^2)} \log Z'(\mathbf{r}) \Big|_{\Phi=0} \quad (200)$$

$$g_R = -\frac{a^3(s + J)^4}{\beta s^4} \frac{\partial^2}{\partial (a^3|\Phi(\mathbf{r})|^2)^2} \log Z'(\mathbf{r}) \Big|_{\Phi=0}. \quad (201)$$

They depend on μ , J , β , and $|\Phi(\mathbf{r})|^2$. Further, we introduce the rescaled order parameter

$$\Phi_R(\mathbf{r}) = \frac{s}{s + J} \Phi(\mathbf{r}). \quad (202)$$

With these coefficients, the full mean-field equation (196) can be approximated by the equation

$$\left[-\frac{Ja^2}{6} \nabla^2 - \mu_R + g_R |\Phi_R(\mathbf{r})|^2 \right] \Phi_R(\mathbf{r}) = 0, \quad (203)$$

This equation has the same form as the conventional stationary GP equation, where μ_R and g_R play the role of a renormalised chemical potential and a renormalised interaction constant, respectively. Their dependence on μ is shown in Fig. 14. Therefore we refer to this equation as a “renormalised GP equation” [72]. The zero temperature limits of the coefficients are calculated in Appendix F.4, see Eq. (248). Near the phase transition to the empty phase, i.e. in the dilute regime, where $\mu = -J + \Delta\mu$, $\Delta\mu \ll J$, we find

$\mu_R = \Delta\mu + \mathcal{O}(\Delta\mu^2)$. Thus, in the limiting case of a dilute BEC and zero temperature, the renormalised GP equation goes over to the conventional GP equation with the interaction parameter $g = g_R = 2a^3J$. While g_R is always positive, μ_R can change sign. A BEC exists if $\mu_R > 0$, otherwise the order parameter vanishes. The phase transition between the BEC and the non-condensate phase is given by the relation $\mu_R = 0$, which is equivalent to Eq. (181) in a translational-invariant system. Inside the BEC phase, μ_R increases linearly with increasing μ , reaches a maximum and decreases again until the condensate is destroyed totally due to strong interaction effects.

6 Discussion

6.1 Comparison of the results

The main results that we found for the one-dimensional model, the paired-fermion model, and the slave-boson model, will be summarized and discussed in this section. All three models give more or less the same physics at zero temperature, with an empty phase, a phase with a particle number per lattice site between 0 and 1, and a Mott insulator. Their common features and differences shall be pointed out in detail.

6.1.1 Phase diagram, total density and condensate density

At zero temperature, the exact solution of the one-dimensional model exhibits three phases in the translational invariant case, as shown in Fig. 6 in the J - μ plane: An empty phase which contains no particles in equilibrium (physically speaking, it costs energy to put a particle into the system), an incommensurate phase with a particle number per lattice site n_{tot} between 0 and 1, and a Mott-insulator with $n_{\text{tot}} = 1$. The same zero-temperature phase diagram has been found for the paired-fermion model (see picture (a) in Fig. 9) and the slave-boson model on the mean-field level. The only difference is that for the three-dimensional models, the incommensurate phase is a BEC, whereas in the case of the one-dimensional model there is no BEC but only a long range correlated phase. This is a consequence of the Mermin-Wagner theorem [8, 9]. At non-zero temperatures, the empty phase and the MI are affected by thermal fluctuations, and they have no clear phase boundary any more. However, the three-dimensional systems still have a single phase boundary between a BEC with a non-zero order parameter, and a non-condensed phase where the order parameter vanishes. The shape of this phase boundary depends on temperature (see picture on the right hand side of Fig. 9 for the paired-fermion model).

For the one dimensional model, the total particle density at $T = 0$ and $T > 0$ is shown in Fig. 5. At $T = 0$, the derivative $\partial n_{\text{tot}} / \partial \mu$ diverges at the phase transitions between the BEC and the empty phase and the BEC and the MI phase. The sharp transitions are “washed out” at finite temperatures.

The zero temperature mean-field results for the total particle density and the condensate density of the paired-fermion model and the slave-boson model agree with each other and are given in the Eqs. (154) and (155). We find a total particle density which increases linearly with μ . In the dilute regime the condensate density is given by $n_0 = n_{\text{tot}} - \mathcal{O}(n_{\text{tot}}^2)$. If we neglect the terms of order n_{tot}^2 , this is in agreement with Gross-Pitaevskii theory which assumes that all particles are condensed in this regime. In the absence of a trapping potential, a solution of the stationary GP equation is given by

$$n_0 = \frac{\mu}{g}. \quad (204)$$

This describes a linearly increasing condensate density n_0 with respect to the chemical potential. Although it takes the repulsion into account by a factor $1/g$ which is decreasing with increasing interaction constant g , the saturation of n_0 cannot be seen in this solution. From the physical point of view, in a realistic description for large densities, the particle density must saturate because there is a finite scattering volume around each particle. Furthermore, for increasing particle density, the condensate density should reach a maximum and for even larger densities, decrease again until its total destruction, because of the increasing

interparticle interaction. This is the behaviour that we found for the slave-boson and the paired-fermion model in mean-field approximation. A similar behaviour has also been found by variational perturbation theory [73], and diffusion Monte Carlo calculations [74]. In order to describe condensates at higher densities, the second order term in the low-density expansion of the energy density has been taken into account which leads to a modified GP theory [4, 74, 75, 76].

At non-zero temperatures the phase boundaries of the empty phase and the MI are not well defined any more, like in the one-dimensional case. The region of BEC shrinks and the condensate density decreases. Non-zero temperature results of the paired-fermion model and the slave-boson model are very similar but not identical (compare the figs. 10 and 13). This is a consequence of the different mean-field approaches. The effect of quantum fluctuations on the zero-temperature result has been studied for the paired-fermion model. A condensate depletion was found, but the critical points were not affected (see Fig. 11).

6.1.2 Excitation spectrum

The spectrum of quasiparticle excitations is found on the level of Gaussian fluctuations. For the paired-fermion model, and the slave-boson model, the expressions for the quasiparticle spectra $E_{\mathbf{k}}$ are summarised in the subsequent table:

$E_{\mathbf{k}}$	in the BEC phase	in the non-condensed phases
paired-fermion model	$\sqrt{\epsilon_{\mathbf{k}} \left[J \left(1 - \left(\frac{\mu}{J} \right)^2 \right) + \left(\frac{\mu}{J} \right)^2 \epsilon_{\mathbf{k}} \right]}$	$\epsilon_{\mathbf{k}} + \mu - J$
slave-boson model	$\sqrt{\epsilon_{\mathbf{k}} \left(2 \frac{(s+J)^2}{s^2} \tilde{a}_4 \Phi_0 ^2 + \epsilon_{\mathbf{k}} \right)}$	$\epsilon_{\mathbf{k}} + (s+J)^2 \tilde{a}_2 / s^2$

Here, $\epsilon_{\mathbf{k}}$ is the free-particle dispersion relation in the optical lattice, given by Eq. (58). We find a spectrum which is linear for small wave vectors \mathbf{k} in the BEC phase, whereas the spectrum has a gap in the non-condensed phases. The gapless spectrum in the BEC phase is caused by a Goldstone mode due to a broken global $U(1)$ symmetry [15]. The result given for the paired-fermion model is only valid at zero temperature. The gapped spectrum is found both in the empty phase and in the MI phase. The result for the slave-boson model depends implicitly on temperature via the coefficients \tilde{a}_2 and \tilde{a}_4 given in Eqs. (185) and (186), and it also depends on the non-physical parameter s .

We have shown that the zero-temperature results of all three models inside the BEC phase and near the phase boundary to the empty phase ($\mu + J \ll J$), agree with the Bogoliubov result

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} (2\mu + \epsilon_{\mathbf{k}})}.$$

The only difference is that the chemical potential is shifted ($\mu \rightarrow \mu + J$), because the phase transition in Bogoliubov theory is given by $\mu = 0$ instead of $\mu = -J$ for the two three-dimensional models. The region near the phase transition to the empty phase is the weakly interacting regime, therefore Bogoliubov theory is applicable there. The interaction constant was identified as $g \equiv 2a^3 J$ (where the lattice constant a was set to 1 in the lattice models).

The gapped spectrum in the MI that was found in the paired-fermion and slave-boson models is of the form

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Delta. \quad (205)$$

We have shown that in the MI phase, near the phase transition to the BEC phase, the gap is given by $\Delta = \mu - J$.

For the one-dimensional system, the excitation spectrum in the incommensurate phase can be found indirectly by means of the Feynman relation and is given in Eq. (99). It is linear for small wave-vectors \mathbf{k} , like in the BEC phase of the three-dimensional systems discussed above.

6.1.3 Static structure factor

The static structure factor is defined as the Fourier transform of the equal-time density-density CF, as it is defined in Eq. (54). At zero temperature it is related to the quasiparticle excitation spectrum via the Feynman relation

$$S(\mathbf{q}) = \frac{Ja^2 \mathbf{q}^2}{2d E_{\mathbf{q}}},$$

where the identification $\hbar^2/2m \equiv Ja^2/2d$ can be considered for a lattice system (in this case $m = m^*$ is the band mass as defined in Eq. (59)). For the weakly interacting Bogoliubov gas the density-density CF was calculated explicitly on the level of a Gaussian approximation. It shows an algebraic decay with $1/r^{d+1}$, where d is the dimension. The result for the static structure factor agrees with the Feynman relation. For the one-dimensional system the density-density CF, and therefore the static structure factor, were calculated exactly in the incommensurate phase, and agree with results from the literature. In the MI phase it vanishes.

6.2 Comparison with results from the Bose-Hubbard model

In previous calculations, performed on the Bose-Hubbard model, each phase requires its own specific mean-field approach [55, 77] or a single one close to the phase boundary [35]. Within a Bogoliubov approximation to the Bose-Hubbard model the quasiparticle spectrum in the BEC phase was found as [55, 77]

$$\epsilon_q = \sqrt{J^2 g_q^2 + 2U n_0 J g_q},$$

where U is the interaction parameter and n_0 is the condensate density. In contrast to this expression, we found for the spectrum the expressions in the table in section 6.1.2. These expressions do not agree in the limit $U \rightarrow \infty$. Thus our hard-core Bose gas cannot be described within the Bogoliubov approximation to the Bose-Hubbard model by simply sending U to infinity. On the other hand, our results are in good agreement with a variational Schwinger-boson mean-field approach to the Bose-Hubbard model, which describe the phases near the phase transition, by sending U to infinity [35]. In the large- U limit of the Bose-Hubbard model, multiple occupation of lattice sites is prohibited because it cost a large amount of energy. Therefore one can assume that in this case, the bosons behave like hard-core bosons.

The results for the excitation spectrum in the Mott-insulating phase from the paired-fermion model and the slave-boson model are consistent with the spectrum that was found for the Bose-Hubbard model in the large- U limit. Inside the first Mott lobe, which is the equivalent to the MI with filling $n_{\text{tot}} = 1$ for hard-core bosons, the latter is given by the expression [55, 70, 35]

$$E_{\mathbf{k}}^{\text{qp/qh}} = \pm \left(-\mu + \frac{U}{2} - \frac{J - \epsilon_{\mathbf{k}}}{2} \right) + \frac{1}{2} \sqrt{(J - \epsilon_{\mathbf{k}})^2 - 6U(J - \epsilon_{\mathbf{k}}) + U^2}, \quad (206)$$

which describes two branches: One (“+” sign) is assigned to quasiparticles and one (“−” sign) to quasiholes. It depends on the interaction parameter U . For our hard-core bosons, only the quasihole branch can exist, because the hard-core condition prohibits multiple occupation of lattice sites, in contrary to the Bose-Hubbard model, where multiple occupation is possible and allows the creation of particle-hole pairs. For large values of U the square root term can be written as

$$\frac{1}{2} \sqrt{(J - \epsilon_{\mathbf{k}})^2 - 6U(J - \epsilon_{\mathbf{k}}) + U^2} = \frac{U}{2} - \frac{3}{2} (J - \epsilon_{\mathbf{k}}) + \mathcal{O}(U^{-1}),$$

such that we find for the two branches the large- U results

$$E_{\mathbf{k}}^{\text{qp}} = \epsilon_{\mathbf{k}} + U - (\mu + 2J) + \mathcal{O}(U^{-1}), \quad (207)$$

$$E_{\mathbf{k}}^{\text{qh}} = \epsilon_{\mathbf{k}} + (\mu - J) + \mathcal{O}(U^{-1}). \quad (208)$$

The gap of the quasiparticle branch is of the order of U , and in the $U \rightarrow \infty$ limit it goes to infinity, because the energy to occupy a site with two particles is infinitely large. On the other hand, the terms which are proportional to U cancel for the quasihole branch, and its $U \rightarrow \infty$ limit is identical to the result given in Eq. (205). Particle-hole excitations cannot be created for hard-core bosons, so the creation of an elementary excitation is associated to removing a particle out of the Mott-insulator. This is possible in the grand-canonical ensemble, where only the average number is fixed but the number of particles fluctuates. Inside the empty phase, the same quasiparticle spectrum was found as for the Mott-insulator, due to the particle-hole symmetry. Here, the creation of an excitation is interpreted by putting an additional particle into the system.

7 Conclusion

In this review, the many-particle problem of strongly interaction bosons in a lattice potential was investigated. This is motivated by recent experiments on Bose-Einstein condensates in optical lattices which showed the phase transition from a BEC to a Mott-insulator. Three different models are discussed, which allow the calculation of the phase diagram, and experimentally observable physical quantities like the total density, the condensate density, the quasiparticle spectrum, and the static structure factor. All these models have in common that they simulate a strong repulsive interaction by imposing a hard-core condition on the bosons, which prohibits a multiple occupation of lattice sites. They are defined by means of the functional integral method.

The first model is a special construction which describes non-interacting impenetrable fermions in a one-dimensional lattice. We exploited the well-known fact that such a fermionic system is equivalent to impenetrable bosons in one dimension, and that the static structure factors of the fermionic and the bosonic system are identical. As the fermions are non-interacting, the model can be integrated out exactly. We calculated the local particle density, the density-density correlation function and the static structure factor in a translational invariant system as well as in a system with a harmonic trap potential. In the translational invariant case, the static structure factor, which is experimentally accessible in Bragg scattering experiments, increases linearly for small wave vectors, until it reaches unity and remains constant. The density-density correlation function shows characteristic oscillations and decays like $1/r^2$.

The other two models were applied on a Bose gas in a three dimensional lattice. They were treated in mean-field theory. The first one, which was called the paired-fermion model, was constructed by a field of pairs of Grassmann variables. It can be seen as an interacting fermionic model. The second one was based on a slave-boson approach. A Hubbard-Stratonovich transformation allows to integrate out the original fields in both models. This transformation leads to new fields, which are connected to the condensate order parameter. A saddle-point approximation provides both a mean-field solution and Gaussian fluctuations. The latter contain the information about quasiparticle excitations. For a three-dimensional lattice, the total particle density and the condensate density can be calculated in mean-field theory, and the quasiparticle spectrum and the static structure factor was calculated on the level of Gaussian fluctuations. The saddle point approximations of the two models lead to qualitatively the same results.

Our results for the one-dimensional model, the paired-fermion model, and the slave-boson model, show a particle hole symmetry. At zero temperature, they have a common phase diagram, with one phase boundary between the empty phase and the incommensurate phase, and one between the incommensurate phase and the Mott-insulating phase. If the temperature is non-zero, there is no clear phase transition between the empty phase and the Mott-insulator due to thermal fluctuations. While there is no Bose-Einstein condensation in the one-dimensional system, the incommensurate phase is a BEC in the paired-fermion and slave-boson model in three dimensions. For the latter two models, the mean-field results for the total density and the condensate density agree exactly at zero temperature, at higher temperature they agree qualitatively. It was shown that they lead to the Gross-Pitaevskii result in the limit of low temperature, if

the density is small compared to the lattice constant. At higher temperatures, we have shown that the slave-boson model leads to a renormalised Gross-Pitaevskii equation with temperature dependent coefficients. A similar theory could in principle be derived on the mean-field level from the paired-fermion model as well. It could be compared to the renormalised Gross-Pitaevskii theory which was derived from the slave-boson model.

The quasiparticle spectra which were found for both three-dimensional models, are gapless (Goldstone mode) in the BEC phase. In the dilute regime, they agree with the well-known Bogoliubov result. In the empty phase and the Mott-insulator, the quasiparticle spectrum is gapped. Our results agree with results which were derived for the Bose-Hubbard model, if the on-site interaction constant U is very large. The Goldstone mode in the BEC phase of the paired-fermion model was found as the quasiparticle pole of only one eigenvalue of the 4×4 quasiparticle Green's function. Additional massive modes may be found from the remaining eigenvalues.

At zero temperature, the elementary excitations are connected to the static structure factor via the Feynman relation. In the empty phase and the Mott-insulator, the static structure factor vanishes because of the absence of density fluctuations.

A Finite sums and products

A.1 Bosonic sum

For bosonic systems, which have a periodic structure in the imaginary time variable, we have to perform sums of the type

$$\sum_{n=1}^M \frac{1}{M} \frac{e^{-\frac{2\pi i}{M}nm}}{1 - a e^{\frac{2\pi i}{M}n}}.$$

This sum is performed by finding the common denominator, which is given by $1 - a^M$. The numerator then is

$$\text{numerator} = \sum_{n=1}^M e^{-\frac{2\pi i}{M}nm} \prod_{k \neq n} \left(1 - a e^{\frac{2\pi i}{M}k}\right)$$

where

$$\prod_{k \neq n} \left(1 - a e^{\frac{2\pi i}{M}k}\right) = \frac{1 - a^M}{1 - a e^{\frac{2\pi i}{M}n}} = 1 + a e^{\frac{2\pi i}{M}n} + a^2 e^{\frac{2\pi i}{M}2n} + \dots + a^{M-1} e^{\frac{2\pi i}{M}(M-1)n}.$$

Therefore we find

$$\begin{aligned} \text{numerator} &= \sum_{n=1}^M e^{-\frac{2\pi i}{M}nm} \sum_{l=1}^M a^{l-1} e^{\frac{2\pi i}{M}(l-1)n} = \sum_{n,l=1}^M a^{l-1} e^{-\frac{2\pi i}{M}n(m-l+1)} = \\ &= M \sum_{l=1}^M a^{l-1} \delta'_{l,m+1}, \quad \text{where } \delta'_{l,k} := \sum_{j=-\infty}^{\infty} \delta_{l,k+jM}. \end{aligned}$$

With the restriction $m = -(M-1), \dots, M-1$ the “enhanced” Kronecker symbol δ' contributes for the two cases

$$\begin{aligned} l &= m+1 & \text{if } m \geq 0 \\ l &= M+m+1 & \text{if } m < 0. \end{aligned}$$

Finally, this leads to the components of the inverse matrix:

$$\sum_{n=1}^M \frac{1}{M} \frac{e^{-\frac{2\pi i}{M}nm}}{1 - a e^{\frac{2\pi i}{M}n}} = \frac{1}{1 - a^M} \times \begin{cases} a^m & \text{if } m \geq 0 \\ a^{M+m} & \text{if } m < 0 \end{cases}. \quad (209)$$

A.2 Fermionic sum

For fermionic systems, which have an anti-periodic structure in the imaginary time variable, we have to perform sums of the type

$$\sum_{n=1}^M \frac{1}{M} \frac{e^{-\frac{2\pi i}{M}(n-\frac{1}{2})m}}{1 - a e^{\frac{2\pi i}{M}(n-\frac{1}{2})}} = \frac{1}{1+a^M} \times \begin{cases} a^m & \text{if } m \geq 0 \\ -a^{M+m} & \text{if } m < 0 \end{cases} . \quad (210)$$

This sum differs from the sum given in Eq. (209) only by the substitution $a \rightarrow a e^{-\pi i m/M}$ and a multiplication by the factor $e^{\pi i m/M}$, so the result can be verified easily.

A.3 Sums with cosines

The following two sums require the condition $|b| > 1$:

$$\sum_{n=1}^M \frac{1}{M} \frac{1}{\cos\left(\frac{2\pi}{M}n\right) - b} = \frac{1}{\sqrt{b^2-1}} \frac{(b - \sqrt{b^2-1})^M + (b + \sqrt{b^2-1})^M + 2}{(b - \sqrt{b^2-1})^M - (b + \sqrt{b^2-1})^M} \quad (211)$$

$$\sum_{n=1}^M \frac{1}{M} \frac{\cos\left(\frac{2\pi}{M}n\right)}{\cos\left(\frac{2\pi}{M}n\right) - b} = \frac{1}{\sqrt{b^2-1}} \frac{(b - \sqrt{b^2-1})^{M-1} + (b + \sqrt{b^2-1})^{M-1} + 2b}{(b - \sqrt{b^2-1})^M - (b + \sqrt{b^2-1})^M} \quad (212)$$

To perform these two sums the following identities were used:

$$\begin{aligned} \frac{1}{\cos(x) - \frac{a^2+1}{2a}} &= \frac{2a^2}{a^2-1} \left[\frac{1}{e^{ix} - a} - \frac{1}{a} \frac{1}{a e^{ix} - 1} \right] \\ \frac{\cos(x)}{\cos(x) - \frac{a^2+1}{2a}} &= \frac{a^2}{a^2-1} \left[\frac{1}{a e^{ix} - 1} - \frac{1}{a} \frac{1}{e^{ix} - a} - \frac{1}{a} \frac{1}{e^{-ix} - a} + \frac{1}{a e^{-ix} - 1} \right] \end{aligned}$$

All separate terms can be traced back to the sum given in Eq. (209).

A.4 Sum for $C(k)$ in Eq. (86)

We perform the sum

$$C(k) = \lim_{M \rightarrow \infty} \sum_{l=1}^M \frac{1}{M} \frac{\left[-e^{\frac{2\pi i}{M}l} + e^{\frac{\pi i}{M}} \left(1 - \frac{\beta}{M} \mu \right) \right] e^{\frac{\pi i}{M}}}{\left(e^{\frac{2\pi i}{M}l} - e^{\frac{\pi i}{M}} \left(1 - \frac{\beta}{M} \mu \right) \right)^2 - e^{\frac{2\pi i}{M}l} e^{\frac{\pi i}{M}} \left(\frac{\beta}{M} J \right)^2 \cos^2 \frac{k}{2}} . \quad (213)$$

Make the following substitutions:

$$\begin{aligned} a &:= - \left(1 - \frac{\beta}{M} \mu \right) e^{\frac{\pi i}{M}} \quad ; \quad b = \frac{\beta}{M} J e^{\frac{\pi i}{2M}} \cos \frac{k}{2} , \\ f(z) &:= \frac{z + a}{(z + a)^2 - b^2 z} . \end{aligned}$$

With these definitions, the sum is given as

$$C(k) = - \lim_{M \rightarrow \infty} \sum_{l=1}^M \frac{1}{M} e^{\frac{\pi i}{M}} f \left(e^{\frac{2\pi i}{M}l} \right) .$$

The roots of the denominator of $f(z)$ are

$$z^{\pm} = \frac{b^2}{2} - a \pm \frac{b}{2} \sqrt{b^2 - 4a}.$$

We perform an expansion into partial fraction and find

$$f(z) = \frac{A}{z - z^+} + \frac{B}{z - z^-} = \frac{(A+B)z - (Az^- + Bz^+)}{(z - z^+)(z - z^-)}$$

with

$$A = \frac{1}{2} + \frac{b}{2\sqrt{b^2 - 4a}} \quad ; \quad B = \frac{1}{2} - \frac{b}{2\sqrt{b^2 - 4a}}.$$

To perform the sum, we use the following identity which can be traced back to Eq. (209):

$$\begin{aligned} \sum_{l=1}^M \frac{1}{M} \frac{1}{e^{\frac{2\pi i}{M}l} - z^{\pm}} &= -\frac{1}{z^{\pm}} \frac{1}{1 - \left(\frac{1}{z^{\pm}}\right)^M} \\ \Rightarrow -\sum_{l=1}^M \frac{1}{M} e^{\frac{\pi i}{M}l} f\left(e^{\frac{2\pi i}{M}l}\right) &= \left[\frac{A}{z^+} \frac{1}{1 - \left(\frac{1}{z^+}\right)^M} + \frac{B}{z^-} \frac{1}{1 - \left(\frac{1}{z^-}\right)^M} \right] e^{\frac{\pi i}{M}}. \end{aligned}$$

The limit $M \rightarrow \infty$ can now be performed, by the help of the identities

$$\begin{aligned} \lim_{M \rightarrow \infty} (z^{\pm})^M &= e^{\pi i} \lim_{M \rightarrow \infty} \left(1 + \left(\pm J \cos \frac{k}{2} - \mu \right) \frac{\beta}{M} + \mathcal{O}\left(\frac{1}{M^2}\right) \right)^M = -e^{\beta(\pm J \cos \frac{k}{2} - \mu)} \\ \lim_{M \rightarrow \infty} z^{\pm} &= 1 \quad ; \quad \lim_{M \rightarrow \infty} A, B = \frac{1}{2}. \end{aligned}$$

The result is given in Eq. (87).

A.5 Sum for G in Eq. (143)

We perform the sum

$$G = \frac{1}{M} \sum_{n=1}^M \frac{i(\varphi_0 + \chi_0)}{1 + (i\varphi_0 + \chi_0)(i\varphi_0^* + \chi_0^*) - 2e^{-\frac{i2\pi}{M}(n-\frac{1}{2})} + \left(1 - \left(\frac{\beta\mu}{2M}\right)^2\right) e^{-2\frac{i2\pi}{M}(n-\frac{1}{2})}}. \quad (214)$$

We define

$$a := 1 + (i\varphi + \chi)(i\varphi^* + \chi^*), \quad b := 1 - \left(\frac{\beta\mu}{2M}\right)^2,$$

$$f(z) = \frac{1}{a - 2z + bz^2}.$$

The roots of the denominator of $f(z)$ are

$$z^{\pm} = \frac{1}{b} \left(1 \pm \sqrt{1 - ab} \right).$$

An expansion into partial fraction leads to

$$f(z) = A \left(\frac{1}{z - z^+} - \frac{1}{z - z^-} \right), \quad \text{where} \quad A = \frac{1}{2\sqrt{1 - ab}}.$$

To perform the sum, we use the following identity which can be traced back to Eq. (210):

$$\begin{aligned} \sum_{l=1}^M \frac{1}{M} \frac{1}{e^{\frac{2\pi i}{M}(l+\frac{1}{2})} - z^\pm} &= -\frac{1}{z^\pm} \frac{1}{1 + \left(\frac{1}{z^\pm}\right)^M} \\ \Rightarrow -\sum_{l=1}^M \frac{1}{M} f\left(e^{\frac{2\pi i}{M}(l+\frac{1}{2})}\right) &= A \left[\frac{1}{z^+} \frac{1}{1 + \left(\frac{1}{z^+}\right)^M} - \frac{1}{z^-} \frac{1}{1 + \left(\frac{1}{z^-}\right)^M} \right]. \end{aligned}$$

A.6 Product to calculate the determinant of Eq. (120)

We want to perform a product of the type

$$\prod_{n=1}^M \left(b - \cos\left(\frac{2\pi}{M}n\right) \right), \quad |b| > 1.$$

This can be verified to be equal to

$$\prod_{n=1}^M \left[\frac{1}{2} \left(b + \sqrt{b^2 - 1} \right) \left(1 - \left(b - \sqrt{b^2 - 1} \right) e^{i\frac{2\pi}{M}n} \right) \left(1 - \left(b - \sqrt{b^2 - 1} \right) e^{-i\frac{2\pi}{M}n} \right) \right],$$

such that the identity

$$\prod_{n=1}^M \left(1 - a e^{\frac{2\pi i}{M}n} \right) = 1 - a^M, \quad (215)$$

can be applied. As a result we find

$$\prod_{n=1}^M \left(b - \cos\left(\frac{2\pi}{M}n\right) \right) = 2^{-M} \left(\left(b + \sqrt{b^2 - 1} \right)^M + \left(b - \sqrt{b^2 - 1} \right)^M - 2 \right). \quad (216)$$

B Coherent states for bosons and fermions

The functional integral representation for bosonic and fermionic systems is constructed of coherent states [36]. We denote bosonic operators by \hat{a}_α^+ , \hat{a}_α , and the fermionic operators by \hat{c}_α^+ , \hat{c}_α . The commutation relations are

$$[\hat{a}_\alpha, \hat{a}_{\alpha'}^+]_- = \delta_{\alpha\alpha'}, \quad (217)$$

$$[\hat{c}_\alpha, \hat{c}_{\alpha'}^+]_+ = \delta_{\alpha\alpha'}. \quad (218)$$

The vacuum state, i.e. the state containing no particle, we call $|0\rangle$. We define coherent states for

- bosons by means of complex field variables ϕ_α^* , ϕ_α :

$$|\phi\rangle = e^{\sum_\alpha \phi_\alpha \hat{a}_\alpha^+} |0\rangle, \quad \langle\phi| = \langle 0| e^{\sum_\alpha \phi_\alpha^* \hat{a}_\alpha}. \quad (219)$$

- fermions by means of conjugate Grassmann variables $\bar{\psi}_\alpha$, ψ_α , where we require, that the Grassmann variables anticommute with the fermionic operators:

$$\begin{aligned} |\psi\rangle &= e^{-\sum_\alpha \psi_\alpha \hat{c}_\alpha^+} |0\rangle = \prod_\alpha (1 - \psi_\alpha \hat{c}_\alpha^+) |0\rangle, \\ \langle\psi| &= \langle 0| e^{\sum_\alpha \bar{\psi}_\alpha \hat{c}_\alpha} = \langle 0| \prod_\alpha (1 + \bar{\psi}_\alpha \hat{c}_\alpha). \end{aligned} \quad (220)$$

For the construction of the coherent state functional integral, the following properties are relevant. They can be checked by using the previous definitions and the integration properties of complex, Grassmannian and nilpotent variables:

- Coherent states are eigenvalues of annihilation operators:

$$\hat{x}_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle, \quad \langle \xi | \hat{x}_\alpha^\dagger = \langle \xi | \bar{\xi}_\alpha, \quad (221)$$

where $\hat{x} = \hat{a}$, $\xi = \phi$, $\bar{\xi} = \phi^*$ for bosons, and $\hat{x} = \hat{c}$, $\xi = \psi$, $\bar{\xi} = \bar{\psi}$ for fermions.

- Scalar product, where the operator \hat{X} is built of bosonic, fermionic, or hard-core operators, respectively:

$$\langle \xi | \hat{X}(\hat{x}^\dagger, \hat{x}) | \xi' \rangle = e^{\sum_\alpha \bar{\xi}_\alpha \xi'_\alpha} X(\bar{\xi}_\alpha, \xi'_\alpha), \quad (222)$$

where \hat{x} , ξ , $\bar{\xi}$ have to be chosen as mentioned above.

- Closure relation (the unity operator is denoted by 1):

$$1 = \int e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} |\phi\rangle \langle \phi| \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \quad (223)$$

$$1 = \int e^{-\sum_\alpha \bar{\psi}_\alpha \psi_\alpha} |\psi\rangle \langle \psi| \prod_\alpha d\bar{\psi}_\alpha d\psi_\alpha. \quad (224)$$

- Trace of an operator \hat{X} :

$$\text{Tr } \hat{X}(\hat{a}_\alpha^\dagger, \hat{a}_\alpha) = \int e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \langle \phi | \hat{X} | \phi \rangle \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \quad (225)$$

$$\text{Tr } \hat{X}(\hat{c}_\alpha^\dagger, \hat{c}_\alpha) = \int e^{-\sum_\alpha \bar{\psi}_\alpha \psi_\alpha} \langle -\psi | \hat{X} | \psi \rangle \prod_\alpha d\bar{\psi}_\alpha d\psi_\alpha. \quad (226)$$

Using these identities, the functional integral of the grand canonical partition function

$$Z = \text{Tr } e^{-\beta(\hat{H}(\hat{x}_\alpha^\dagger, \hat{x}_\alpha) - \mu \hat{N}(\hat{x}_\alpha^\dagger, \hat{x}_\alpha))}$$

with the Hamiltonian \hat{H} is constructed in the following manner: We apply the relation for the trace and insert the closure relation $M - 1$ times. Introducing the discrete-imaginary-time index $n = 1, \dots, M$ we have

$$Z = \int e^{\sum_{\alpha,n} \bar{\xi}_{\alpha,n} \xi_{\alpha,n}} \langle \sigma \bar{\xi}_1 | e^{-\frac{\beta}{M}(\hat{H} - \mu \hat{N})} | \xi_M \rangle \prod_{n=2}^M \langle \bar{\xi}_n | e^{-\frac{\beta}{M}(\hat{H} - \mu \hat{N})} | \xi_{n-1} \rangle \prod_{\alpha,n} \frac{d\bar{\xi}_\alpha d\xi_\alpha}{\mathcal{N}}, \quad (227)$$

where $\sigma = +1$ for bosons and -1 for fermions, and $\mathcal{N} = 2\pi i$ for bosons and 1 for fermions. The minus sign inside the scalar product in the fermionic trace gives rise to the anti-periodicity of the fermionic field variables. The different sign in the exponent of the hard-core bosonic trace is the reason that the diagonal term in the action for hard-core bosons is different from bosonic and fermionic actions.

The operator in the exponent $\hat{H}(\hat{x}_\alpha^\dagger, \hat{x}_\alpha) - \mu \hat{N}(\hat{x}_\alpha^\dagger, \hat{x}_\alpha)$ can be replaced by its normal ordered form by making an error of the order $(\beta/M)^2$ which vanishes for $M \rightarrow \infty$. Applying the eigenvalue property and the product property yields

$$Z = \lim_{M \rightarrow \infty} \int e^{-A(\bar{\xi}, \xi)} \prod_{n=1}^M \prod_\alpha \frac{d\bar{\xi}_{\alpha,n} d\xi_{\alpha,n}}{\mathcal{N}} \quad (228)$$

with the action

$$A(\bar{\xi}, \xi) = \frac{\beta}{M} \sum_{n=1}^M \left\{ \sum_{\alpha} \sigma_1 \bar{\xi}_{\alpha, n+1} \left[\frac{M}{\beta} (\xi_{\alpha, n+1} - \xi_{\alpha, n}) - \mu \xi_{\alpha, n} \right] + H(\xi_{\alpha, n+1}^*, \xi_{\alpha, n}) \right\} \quad (229)$$

and the boundary condition $\xi_{\alpha, 1} = \sigma_2 \xi_{\alpha, M+1}$, $\bar{\xi}_{\alpha, 1} = \sigma_2 \bar{\xi}_{\alpha, M+1}$.

C Expectation values and Wick's theorem

An expectation value of an expression in terms of real/complex/Grassmann variables is defined by means of Eq. (41). A *second order expectation value* provides the matrix element of the (inverse) Green's matrix $\hat{\mathcal{G}}$:

$$\begin{aligned} \text{Real variables:} & \quad \langle \phi_j \phi_k \rangle = \frac{1}{2} \hat{\mathcal{G}}_{jk}^{-1} \\ \text{Complex conjugate variables:} & \quad \langle \phi_j^* \phi_k \rangle = \hat{\mathcal{G}}_{jk}^{-1} \\ \text{Conjugate Grassmann variables:} & \quad \langle \bar{\psi}_j \psi_k \rangle = \hat{\mathcal{G}}_{jk} \end{aligned} \quad (230)$$

Forth order expectation values can be calculated via the application of Wick's theorem [14, 36]. It can be split into products of second-order expectation values and a sum has to be performed over all possible pairings (including a sign for Grassmann variables):

$$\begin{aligned} \text{Real var.:} & \quad \langle \phi_j \phi_k \phi_l \phi_m \rangle = \langle \phi_j \phi_k \rangle \langle \phi_l \phi_m \rangle + \langle \phi_j \phi_l \rangle \langle \phi_k \phi_m \rangle + \langle \phi_j \phi_m \rangle \langle \phi_k \phi_l \rangle \\ \text{C. conj. var.:} & \quad \langle \phi_j^* \phi_k^* \phi_l \phi_m \rangle = \langle \phi_j^* \phi_m \rangle \langle \phi_k^* \phi_l \rangle + \langle \phi_j^* \phi_l \rangle \langle \phi_k^* \phi_m \rangle \\ \text{Conj. Gr. var.:} & \quad \langle \bar{\psi}_j \bar{\psi}_k \bar{\psi}_l \bar{\psi}_m \rangle = \langle \bar{\psi}_j \bar{\psi}_m \rangle \langle \bar{\psi}_k \bar{\psi}_l \rangle - \langle \bar{\psi}_j \bar{\psi}_l \rangle \langle \bar{\psi}_k \bar{\psi}_m \rangle \end{aligned} \quad (231)$$

D Correlations

The decay of the density-density CF given in Eq. (129) is investigated in $d = 1, 2, 3$ dimensions. For convenience we write $c := \sqrt{2(\mu + J)}$. We use a cut-off at $|\mathbf{q}| = Q$ for the integrals.

- **One dimension:**

$$D(r) = \int_{-Q}^Q \frac{|q|}{c} e^{iqr} dq = \frac{2}{cr^2} \int_0^{Qr} q' \cos(q') dq' \sim \frac{1}{r^2}$$

The anti-symmetrical part which is $\sim \sin(q')$ does not contribute.

- **Two dimensions** with polar coordinates (q, ϕ) :

$$D(r) = \int_0^Q dq q \int_0^{2\pi} d\phi \frac{q}{c} e^{iqr \cos \phi} = \frac{1}{cr^3} \int_0^{2\pi} d\phi \frac{1}{\cos^3 \phi} \int_0^{rQ} q'^2 \cos(q') dq' \sim \frac{1}{r^3}$$

- **Three dimensions** with spherical coordinates (q, θ, ϕ) :

$$\begin{aligned} D(r) &= \int_0^Q dq q^2 \int_0^{2\pi} d\phi \int_1^{-1} d(\cos \theta) \frac{q}{c} e^{iqr \cos \theta} \\ &= \frac{2\pi}{cr^3} \int_1^{-1} d(\cos \theta) \frac{1}{\cos^4 \theta} \int_0^{rQ} q'^3 \cos(q') dq' \sim \frac{1}{r^4} \end{aligned}$$

E Calculations to the paired-fermion model

In this Appendix we write out the expression for the Green's function in both cases $|\phi| = 0$ and $|\phi| \neq 0$.

Case: $|\phi| = 0$

Deviation of the effective action due to fluctuations is

$$\delta A_{\text{eff}} = \sum_{\mathbf{k}, \omega} \begin{pmatrix} \delta \phi_{\mathbf{k}, \omega} & \delta \chi_{\mathbf{k}, \omega} \end{pmatrix} \overbrace{\begin{pmatrix} v_{\mathbf{k}}^{-1} - D(\omega) & iD(\omega) \\ iD(\omega) & \frac{1}{2J} + D(\omega) \end{pmatrix}}^{\hat{\mathcal{G}}^{-1}} \begin{pmatrix} \delta \phi_{\mathbf{k}, \omega}^* \\ \delta \chi_{\mathbf{k}, \omega}^* \end{pmatrix}, \quad (232)$$

where

$$D(\omega) = \frac{1}{|\mu| - i\omega}, \quad v_{\mathbf{k}}^{-1} = \frac{1}{J(3 - \epsilon_{\mathbf{k}})}.$$

The determinant of the Green's function reads

$$\det \hat{\mathcal{G}}^{-1} = \frac{v_{\mathbf{k}}^{-1}}{2J} - D(\omega) \left(\frac{1}{2J} - v_{\mathbf{k}}^{-1} \right). \quad (233)$$

Case: $|\phi| \neq 0$

Deviation of the effective action due to fluctuations is

$$\delta A_{\text{eff}} = \sum_{\mathbf{k}, \omega} \begin{pmatrix} \delta \phi_{\mathbf{k}, \omega} & \delta \chi_{\mathbf{k}, \omega} & \delta \phi_{-\mathbf{k}, -\omega}^* & \delta \chi_{-\mathbf{k}, -\omega}^* \end{pmatrix} \hat{\mathcal{G}}^{-1} \begin{pmatrix} \delta \phi_{\mathbf{k}, \omega}^* \\ \delta \chi_{\mathbf{k}, \omega}^* \\ \delta \phi_{-\mathbf{k}, -\omega} \\ \delta \chi_{-\mathbf{k}, -\omega} \end{pmatrix} \quad (234)$$

with the Green's function

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} v_{\mathbf{k}}^{-1} - D(\omega) & iD(\omega) & -a & ia \\ iD(\omega) & \frac{1}{2J} + D(\omega) & ia & a \\ -a & ia & v_{\mathbf{k}}^{-1} - D(\omega) & iD(\omega) \\ ia & a & iD(\omega) & \frac{1}{2J} + D(\omega) \end{pmatrix}, \quad (235)$$

where

$$D(\omega) = \frac{1}{2} \cdot \frac{\mu^2 + J^2 + 2i\mu\omega}{J(J^2 + \omega^2)},$$

$$D(-\omega) = \frac{1}{2} \cdot \frac{\mu^2 + J^2 - 2i\mu\omega}{J(J^2 + \omega^2)},$$

$$a = -\frac{1}{2} \cdot \frac{|\Phi|^2/9}{J(J^2 + \omega^2)}.$$

The determinant of the Green's function is

$$\det \hat{\mathcal{G}}^{-1} = \frac{1}{[2J^2(3 - \epsilon_{\mathbf{k}})]^2(J^2 + \omega^2)} \cdot [\omega^2 + (J^2 - \mu^2)\epsilon_{\mathbf{k}} + \mu^2\epsilon_{\mathbf{k}}^2]. \quad (236)$$

F Calculations to the slave-boson model

F.1 Integration of the constraint

We perform the integration of the complex fields b and e . The integral factorises such that it can be performed for each lattice site \mathbf{r} independently. Therefore we will drop the index \mathbf{r} here temporarily and evaluate the expression

$$\int \exp \left\{ -\beta s \varphi^2 - \beta(e, b) \begin{pmatrix} 2s\varphi + s & s\Phi \\ s\Phi^* & -\mu \end{pmatrix} \begin{pmatrix} e^* \\ b^* \end{pmatrix} \right\} \delta(|b|^2 + |e|^2 - 1) de^* de db^* db. \quad (237)$$

The eigenvalues of the 2×2 matrix are

$$\lambda_{\pm} = \beta s \left(\varphi + \frac{1}{2} \right) - \beta \frac{\mu}{2} \pm \beta \sqrt{\left[\left(\varphi + \frac{1}{2} \right) s + \frac{\mu}{2} \right]^2 + s^2 |\Phi|^2}.$$

A unitary transformation can be applied to the vector (e, b) such that the matrix has diagonal form. This does not affect the constraint, because the expression $|b|^2 + |e|^2 = 1$ remains unchanged after a unitary transformation. Therefore the integral is equal to

$$\begin{aligned} & \int de^* de db^* db \exp \left[-\beta s \varphi^2 - \lambda_1 |e|^2 - \lambda_2 |b|^2 \right] \delta(|b|^2 + |e|^2 - 1) \\ &= (2\pi)^2 \frac{1}{2} \int_0^1 d\rho \rho \exp \left[-\beta s \varphi^2 - \lambda_1 \rho^2 - \lambda_2 (1 - \rho^2) \right] \\ &= 2\pi^2 e^{-\beta s \varphi^2} \frac{e^{-\lambda_1} - e^{-\lambda_2}}{\lambda_1 - \lambda_2} \\ &= 4\pi^2 \exp \left[-\beta s \varphi^2 - \beta s \left(\varphi + \frac{1}{2} \right) + \beta \frac{\mu}{2} \right] \frac{\sinh \left[\beta \sqrt{\left[\left(\varphi + \frac{1}{2} \right) s + \frac{\mu}{2} \right]^2 + s^2 |\Phi|^2} \right]}{\beta \sqrt{\left[\left(\varphi + \frac{1}{2} \right) s + \frac{\mu}{2} \right]^2 + s^2 |\Phi|^2}}. \end{aligned}$$

After performing the shift $\varphi + 1/2 \rightarrow \varphi$ and using the index \mathbf{r} again, the integral (237) gives the result

$$\int_{-\infty}^{\infty} d\varphi_{\mathbf{r}} \frac{\sinh \left[\beta \sqrt{\left(\varphi_{\mathbf{r}} s + \frac{\mu_{\mathbf{r}}}{2} \right)^2 + s^2 |\Phi_{\mathbf{r}}|^2} \right]}{\beta \sqrt{\left(\varphi_{\mathbf{r}} s + \frac{\mu_{\mathbf{r}}}{2} \right)^2 + s^2 |\Phi_{\mathbf{r}}|^2}} e^{-\beta s \varphi_{\mathbf{r}}^2 + \frac{\beta \mu_{\mathbf{r}}}{4}}. \quad (238)$$

F.2 Condensate density

In a Bose system in an optical lattice, which is described by a complex field $\phi_{\mathbf{r}}(\tau)$, the condensate density is defined by the expression (52) via the concept of off-diagonal long range order. In classical approximation, the field does not depend on imaginary time τ , and in the slave-boson approach, we replace

$$\phi_{\mathbf{r}}^* \rightarrow b_{\mathbf{r}}^* e_{\mathbf{r}}; \quad \phi_{\mathbf{r}} \rightarrow e_{\mathbf{r}}^* b_{\mathbf{r}},$$

thus we use the definition

$$n_0 = \lim_{\mathbf{x} - \mathbf{x}' \rightarrow \infty} \langle b_{\mathbf{x}}^* e_{\mathbf{x}} e_{\mathbf{x}'}^* b_{\mathbf{x}'} \rangle. \quad (239)$$

for the condensate density. Here, the expectation value is given by

$$\langle \dots \rangle = \frac{1}{Z_{\text{sb}}} \int \dots \exp[\dots] \mathcal{D}[\Phi^*, \Phi, \varphi] \mathcal{D}[b, b^*, e, e^*]. \quad (240)$$

We are interested in the connection between the correlation function $\langle \Phi_{\mathbf{x}} \Phi_{\mathbf{x}'}^* \rangle$ and the condensate density. For this purpose we integrate out the field Φ to transform the correlation function of the field Φ back to a correlation function of the fields b and e . Therefore, we write

$$\hat{v}_{\mathbf{r}\mathbf{r}'} := \frac{s\delta_{\mathbf{r}\mathbf{r}'} - \hat{J}_{\mathbf{r}\mathbf{r}'}}{s^2}$$

for simplicity and perform the integration

$$\begin{aligned} & \beta^2 s^2 \int \Phi_{\mathbf{x}} \Phi_{\mathbf{x}'}^* \exp \left[\beta \sum_{\mathbf{r}, \mathbf{r}'} \Phi_{\mathbf{r}}^* \hat{v}_{\mathbf{r}\mathbf{r}'}^{-1} \Phi_{\mathbf{r}'} + \beta s \sum_{\mathbf{r}} \Phi_{\mathbf{r}} b_{\mathbf{r}}^* e_{\mathbf{r}} + \beta s \sum_{\mathbf{r}} \Phi_{\mathbf{r}}^* e_{\mathbf{r}}^* b_{\mathbf{r}} \right] \prod_{\mathbf{r}} d\Phi_{\mathbf{r}} d\Phi_{\mathbf{r}}^* = \\ & \frac{\partial}{\partial(b_{\mathbf{x}}^* e_{\mathbf{x}})} \frac{\partial}{\partial(b_{\mathbf{x}'}^* e_{\mathbf{x}'})} \int \exp \left[\beta \sum_{\mathbf{r}, \mathbf{r}'} \Phi_{\mathbf{r}}^* \hat{v}_{\mathbf{r}\mathbf{r}'}^{-1} \Phi_{\mathbf{r}'} + \beta s \sum_{\mathbf{r}} \Phi_{\mathbf{r}} b_{\mathbf{r}}^* e_{\mathbf{r}} + \beta s \sum_{\mathbf{r}} \Phi_{\mathbf{r}}^* e_{\mathbf{r}}^* b_{\mathbf{r}} \right] \prod_{\mathbf{r}} d\Phi_{\mathbf{r}} d\Phi_{\mathbf{r}}^* = \\ & \frac{\partial}{\partial(b_{\mathbf{x}}^* e_{\mathbf{x}})} \frac{\partial}{\partial(b_{\mathbf{x}'}^* e_{\mathbf{x}'})} \det \left(\frac{\hat{v}}{\beta} \right) \exp \left[\beta s^2 \sum_{\mathbf{r}, \mathbf{r}'} b_{\mathbf{r}}^* e_{\mathbf{r}} \hat{v}_{\mathbf{r}\mathbf{r}'} e_{\mathbf{r}'}^* b_{\mathbf{r}'} \right] = \\ & \beta s^2 \det \left(\frac{\hat{v}}{\beta} \right) \left[\hat{v}_{\mathbf{x}\mathbf{x}'} + \beta s^2 \sum_{\mathbf{r}, \mathbf{r}'} b_{\mathbf{r}}^* e_{\mathbf{r}} e_{\mathbf{r}'}^* b_{\mathbf{r}'} \hat{v}_{\mathbf{r}\mathbf{x}} \hat{v}_{\mathbf{x}'\mathbf{r}'} \right] \exp \left[\beta s^2 \sum_{\mathbf{r}, \mathbf{r}'} b_{\mathbf{r}}^* e_{\mathbf{r}} \hat{v}_{\mathbf{r}\mathbf{r}'} e_{\mathbf{r}'}^* b_{\mathbf{r}'} \right]. \end{aligned}$$

Since we are interested in the limit $\mathbf{x} - \mathbf{x}' \rightarrow \infty$, and the matrix $\hat{J}_{\mathbf{x}\mathbf{x}'}$ includes nearest-neighbour hopping only, the term $\hat{v}_{\mathbf{x}\mathbf{x}'}$ vanishes. This yields for far distant lattice sites \mathbf{x}, \mathbf{x}' the expression

$$\langle \Phi_{\mathbf{x}}^* \Phi_{\mathbf{x}'} \rangle = s^2 \sum_{\mathbf{r}, \mathbf{r}'} \langle b_{\mathbf{r}}^* e_{\mathbf{r}} e_{\mathbf{r}'}^* b_{\mathbf{r}'} \rangle \hat{v}_{\mathbf{r}\mathbf{x}} \hat{v}_{\mathbf{x}'\mathbf{r}'}.$$

Further we can assume that $\langle b_{\mathbf{r}}^* e_{\mathbf{r}} e_{\mathbf{r}'}^* b_{\mathbf{r}'} \rangle = \langle b_{\mathbf{x}}^* e_{\mathbf{x}} e_{\mathbf{x}'}^* b_{\mathbf{x}'} \rangle$ for \mathbf{r}, \mathbf{x} and \mathbf{r}', \mathbf{x}' nearest neighbours. Using

$$\sum_{\mathbf{r}} \hat{v}_{\mathbf{r}\mathbf{x}} = \sum_{\mathbf{r}'} \hat{v}_{\mathbf{x}'\mathbf{r}'} = \frac{s + J}{s^2},$$

we get

$$\lim_{\mathbf{x} - \mathbf{x}' \rightarrow \infty} \langle \Phi_{\mathbf{x}}^* \Phi_{\mathbf{x}'} \rangle = \frac{(s + J)^2}{s^2} \lim_{\mathbf{x} - \mathbf{x}' \rightarrow \infty} \langle b_{\mathbf{x}}^* e_{\mathbf{x}} e_{\mathbf{x}'}^* b_{\mathbf{x}'} \rangle$$

and therefore

$$n_0 = \frac{s^2}{(s + J)^2} \lim_{\mathbf{x} - \mathbf{x}' \rightarrow \infty} \langle \Phi_{\mathbf{x}}^* \Phi_{\mathbf{x}'} \rangle.$$

F.3 Total particle density

The total particle density at site \mathbf{r} is given as

$$n_{\mathbf{r}} = 1 - \langle |e_{\mathbf{r}}|^2 \rangle, \quad (241)$$

where e is the field associated to empty sites. It is possible to express the expectation value of the complex field e in terms of an expectation value of the real field φ . To achieve that, let us regard the integration over the fields b, e , and φ . After performing the substitution $\varphi + 1/2 \rightarrow \varphi$ and dropping the index \mathbf{r} , we have

$$\int d\varphi e^{-\beta s(\varphi - \frac{1}{2})^2} \int \mathcal{D}[b, b^*, e, e^*] |e|^2 \exp \left\{ -\beta(e, b) \begin{pmatrix} 2s\varphi & s\Phi \\ s\Phi^* & -\mu \end{pmatrix} \begin{pmatrix} e^* \\ b^* \end{pmatrix} \right\}$$

$$= -\frac{1}{2s\beta} \int d\varphi e^{-\beta s(\varphi - \frac{1}{2})^2} \frac{\partial}{\partial \varphi} \int \mathcal{D}[b, b^*, e, e^*] \exp \left\{ \dots \right\}.$$

Partial integration leads to

$$\frac{1}{2s\beta} \int d\varphi \left[-2\beta s \left(\varphi - \frac{1}{2} \right) \right] e^{-\beta s(\varphi - \frac{1}{2})^2} \int \mathcal{D}[b, b^*, e, e^*] \exp \left\{ \dots \right\}.$$

Therefore we find

$$\langle |e|^2 \rangle = \left\langle - \left(\varphi - \frac{1}{2} \right) \right\rangle.$$

Together with Eq. (241) we find for the local total particle density the expression

$$n_{\mathbf{r}} = \langle \varphi_{\mathbf{r}} \rangle + \frac{1}{2}. \quad (242)$$

F.4 Zero temperature limit

We want to integrate out the function Z' (we drop the index \mathbf{r}) given in Eq. (176) for zero temperature, i.e. in the limit $\beta \rightarrow \infty$. For simplicity we write $\tilde{\beta} := \beta s$ and perform the limit $\beta \rightarrow \infty$ instead. Further we write $a := \mu/2s$, and $x := |\Phi|^2$. The function Z' we write as

$$Z' = \frac{1}{2\tilde{\beta}} (Z_- - Z_+),$$

where

$$Z_{\pm} = \int_{-\infty}^{\infty} \frac{e^{-\tilde{\beta} f_{\pm}(\varphi, x)}}{\sqrt{(\varphi + a)^2 + x}} d\varphi$$

and

$$f_{\pm}(\varphi, x) = \varphi^2 \pm \sqrt{(\varphi + a)^2 + x}.$$

In the limit $\tilde{\beta} \rightarrow \infty$ we can calculate the φ -integral Z_{\pm} exactly by means of a saddle-point integration. This is done by expanding the functions f_{\pm} in second order about their minimum with respect to φ . We need partial derivatives

$$\begin{aligned} \frac{\partial f_{\pm}(\varphi, x)}{\partial \varphi} &= 2\varphi \pm \frac{\varphi + a}{\sqrt{(\varphi + a)^2 + x}} \\ \frac{\partial^2 f_{\pm}(\varphi, x)}{\partial \varphi^2} &= 2 \pm \frac{x}{[(\varphi + a)^2 + x]^{\frac{3}{2}}}. \end{aligned}$$

We determine the extrema of f_{\pm} :

$$\frac{\partial f_{\pm}(\varphi_0, x)}{\partial \varphi} = 0 \quad \Rightarrow \quad \sqrt{(\varphi_0 + a)^2 + x} = \mp \frac{\varphi_0 + a}{2\varphi_0}, \quad (243)$$

which is equivalent to

$$x = (\varphi_0 + a)^2 \left(\frac{1}{4\varphi_0^2} - 1 \right). \quad (244)$$

Thus the saddle point approximation for large values of $\tilde{\beta}$ is

$$Z_{\pm} \approx \int_{-\infty}^{\infty} \frac{e^{-\tilde{\beta} \left[f_{\pm}(\varphi_0, x) + \frac{1}{2} \frac{\partial^2 f_{\pm}}{\partial \varphi^2}(\varphi_0, x) (\varphi - \varphi_0)^2 \right]}}{\sqrt{(\varphi_0 + a)^2 + x}} d\varphi$$

$$= \sqrt{\frac{\pi}{(\varphi_0 + a)^2 + x}} \frac{e^{-\tilde{\beta} f_{\pm}(\varphi_0, x)}}{\sqrt{\frac{\tilde{\beta}}{2} \frac{\partial^2 f_{\pm}(\varphi_0, x)}{\partial \varphi^2}}}.$$

From Eq. (243) we get

$$f_{\pm}(\varphi_0) = \varphi_0^2 - \frac{1}{2} - \frac{a}{2\varphi_0}; \quad \frac{\partial^2 f_{\pm}(\varphi_0)}{\partial \varphi^2} = 2 - \frac{8x(\varphi_0)\varphi_0^3}{(\varphi_0 + a)^3},$$

where x itself depends on φ_0 independently via Eq. (244). For given x there are two solutions for φ_0 , but only the one which is the absolute minimum contributes to Z' for large values of $\tilde{\beta}$. Therefore:

$$\log Z' = \log(\varphi_0) - \log(\varphi_0 + a) - \frac{1}{2} \log \left(\frac{\partial^2 f_{\pm}(\varphi_0)}{\partial \varphi^2} \right) - \tilde{\beta} f_{\pm}(\varphi_0) + \text{const}.$$

The term that is proportional to $\tilde{\beta}$ dominates all the others, and in the limit $\tilde{\beta} \rightarrow \infty$ we find the *exact* result

$$\begin{aligned} \lim_{\tilde{\beta} \rightarrow \infty} \frac{1}{\tilde{\beta}} \log Z' &= -f_{\pm}(\varphi_0) \\ \Rightarrow \lim_{\tilde{\beta} \rightarrow \infty} \frac{1}{\tilde{\beta}} \frac{\partial}{\partial x} \log Z' &= - \left[\frac{df_{\pm}(\varphi_0)}{d\varphi_0} \right] \frac{d\varphi_0}{dx}. \end{aligned}$$

The derivative of φ_0 with respect to x we get from Eq. (244) by means of the implicit function theorem:

$$\frac{d\varphi_0}{dx} = \frac{-2\varphi_0^3}{(\varphi_0 + a)(4\varphi_0^3 + a)}.$$

Therefore:

$$\lim_{\tilde{\beta} \rightarrow \infty} \frac{1}{\tilde{\beta}} \frac{\partial}{\partial x} \log Z' = \frac{\varphi_0}{\varphi_0 + a}.$$

Together with the mean-field equation (181), we find the zero temperature result in the condensed phase (i.e. where $x > 0$):

$$\frac{s}{s+J} - \frac{\varphi_0}{\varphi_0 + a} = 0 \quad \Rightarrow \quad \varphi_0 = \frac{\mu}{2J}.$$

For the order parameter we find from Eq. (244) in the condensed phase:

$$|\Phi|^2 = x = \frac{1}{4} \left(\frac{s+J}{J_s} \right)^2 (J^2 - \mu^2).$$

Thus the condensate density by the definition in Eq. (177) is:

$$n_0 = \frac{s^2}{(s+J)^2} |\Phi|^2 = \begin{cases} \frac{1}{4} \left(1 - \frac{\mu^2}{J^2} \right) & \text{if } -J < \mu < J \\ 0 & \text{else,} \end{cases} \quad (245)$$

and because of $\langle \varphi \rangle = \varphi_0$ the total particle density by the definition (178) is:

$$n_{\text{tot}} = \varphi_0 + \frac{1}{2} = \begin{cases} 0 & \text{if } \mu \leq -J \\ \frac{1}{2} \left(1 - \frac{\mu}{J} \right) & \text{if } -J < \mu < J \\ 1 & \text{if } J \leq \mu. \end{cases} \quad (246)$$

To determine the coefficient \tilde{a}_4 in Eq. (186), we need the second derivative of $\log Z$ with respect to x :

$$\begin{aligned} \lim_{\tilde{\beta} \rightarrow \infty} \frac{1}{\tilde{\beta}} \frac{\partial^2}{\partial x^2} \log Z' &= \left[\frac{d}{d\varphi} \lim_{\tilde{\beta} \rightarrow \infty} \frac{1}{\tilde{\beta}} \frac{\partial}{\partial x} \log Z' \right] \frac{d\varphi_0}{dx}, \\ &= \frac{1}{s} \frac{-\mu\varphi_0^3}{(\varphi_0 + a)^3 (4\varphi_0^3 + a)}. \end{aligned}$$

With the above solution this yields

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \frac{\partial^2}{\partial x^2} \log Z' = 2J \frac{s^4}{(s+J)^4} \left[1 - 4 \frac{s}{s+J} n_0 \right]. \quad (247)$$

With these results we also find the zero temperature expressions for the renormalised coefficients (200) and (201):

$$\mu_R = -(s+J) + \frac{(s+J)^2}{s+|\mu|}; \quad g_R = 2a^3 J. \quad (248)$$

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